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TECHNICAL ABSTRACTS

THERMAL ANALYSIS OF NTO: COMPETITIVE SUBLIMATION AND CONDENSED PHASE DECOMPOSITION OF A HIGH EXPLOSIVE

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Thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC) experiments have shown that the heating of 3-nitro-1,2,4-triazol-5-one (NTO) causes both sublimation and condensed phase exothermic decomposition. Using model-free isoconversional analysis, global activation energies have been determined as a function of the extent of conversion, α. Sublimation of NTO predominates in an open pan. Nonisothermal TGA and DSC traces strongly support competitive sublimation and condensed phase decomposition for pierced pan samples. Condensed phase decomposition promotes the formation of gaseous reaction products when confining NTO in a closed pan. Activation energies of closed pan samples remain relatively constant at about 310 kJ mol^{-1} for $0.2<\alpha<0.8$.

THERMAL DECOMPOSITION OF A HIGH EXPLOSIVE: COMPETITIVE VAPORIZATION AND DECOMPOSITION OF LIQUID RDX

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Thermogravimetric analysis and differential scanning calorimetry have been applied to the thermal decomposition of hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX). Model-free isoconversional kinetic analysis has been used to determine activation energies as a function of the extent of conversion. Evaporation is a prevalent process in an open pan with an activation energy of about 100 kJ mol^{-1}. Liquid phase decomposition of RDX is promoted by confining the system in either a pierced pan or a closed pan and occurs with an activation energy of about 200 kJ mol^{-1}, which is consistent with scission of an N-N bond as the primary decomposition step. Gas phase decomposition also competes in such a confined environment with an activation energy estimated to be about 140 kJ mol^{-1}. The integrated heat release from RDX is about 500 kJ mol^{-1} in closed pan samples, independent of both the heating rate and the initial sample mass.

SPIN-ORBIT COUPLING AND CHEMI-IONIZATION OF Hg + Hg**

J.S. Cohen, L.A. Collins and R.L. Martin, Los Alamos National Laboratory (Presented at the *Division of Atomic, Molecular and Optical Physics 2000 Meeting of the American Physical Society*, Held in Storrs CT, June 2000).

Chemi-ionization in binary collisions of mercury atoms is possible only when both atoms are excited. We have performed ab initio calculations of a complete set of 36 potential curves ($^{1,3,5}\Sigma,\Pi,\Delta_{g,u}$) for the interactions Hg(6s6p) + Hg(6s6p) as well as the molecular-ion potential curve dissociating to $Hg(6s^2) + Hg^+$. These calculations utilize relativistic core potentials and full configuration interaction involving the valence electrons. The spin-orbit coupled set of 90 potential curves is then obtained by diagonalizing the matrices containing these L-S potential curves and the atomic spin-orbit matrix elements. The attractive or repulsive nature of the curves and their R-dependent position relative to the molecular-ion curve show the possibilities for both associative ionization (yielding vibrationally excited Hg_2^+)and Penning ionization (yielding Hg^+ and ground state Hg). The calculated structure sheds light on some previous puzzling experimental observations.

TROPOSPHERIC OZONE FORMATION FROM BIOMASS BURNING AND URBAN RELEASES

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Atmospheric release of oxidizable carbon compounds, coupled with NO_x release and solar ultraviolet radiation, leads to formation of tropospheric ozone. Ground level ozone data indicate substantial increases over the past century, especially during summer. In urban areas, automotive traffic is a major contributor to ozone formation, although liquefied petroleum gas is also important in cities (for example Mexico City, Santiago). Elevated concentrations of hydrocarbons are also found in cities such as Karachi which depend heavily on traditional local energy sources. The burning of agricultural wastes or forests produces CO, and many hydrocarbons whose yields correlate more closely with CO than with CO_2. Carbonaceous molecular products containing oxygen, nitrogen, sulfur or halogens are present in very fresh plumes. In several aircraft-based Pacific programs, back-trajectories of ozone-rich plumes have been traced thousands of miles to source areas. Relative enhancements of products with different lifetimes are markers of plume ages.

THE KINETIC NATURE OF SULFUR'S CHEMISTRY IN FLAMES

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Radi et al. recently presented the first quantitative multiplexed measurements of S_2 and OH concentrations in flames using degenerate four wave mixing (DFWM). Although the absorption-calibrated OH measurements were in agreement with expectations, very severe discrepancies were reported for the indirectly-calibrated S_2 densities. Magnitudes ranged up to 236-fold larger than predicted. The researchers have questioned the adequacy of previous flame work and the current kinetic model of the mechanisms of sulfur's flame chemistry. The implications of their suggestion are extensive and severe, and their result unexpected. They have suggested that the kinetic modeling is either incomplete or that an additional species such as NS may be responsible. As a consequence, a re-examination of their work and all previous studies in H_2, C_3H_8 and CH_3OH flames has been made. The resulting conclusions are that it will be very difficult to modify the kinetic model of sulfur in flames to encompass such results. Suggestions that other species such as NS may be playing a significant role are shown to have little merit. In addition, an analysis of potential roles for

OCS, CS, CS_2 and one recently suggested for HCS in fossil fueled flames also indicates these to be very minor.

A closer examination of the recent DFWM measurements implies various other disquieting aspects. One is that the reported S_2 densities are essentially close to or above expected flame equilibrium values. Numerous independent measurements all agree that S_2 concentrations are depressed by flame non-equilibrium and increase with downstream time as flame radical concentrations relax towards their equilibrium values. In the present case, however, measured OH concentrations still are in the range of 42- to 10-fold above their equilibrium values. A second aspect of concern is that the measurements imply an insensitivity to S_2, recording levels at several hundreds of ppm with some difficulty. Other DFWM measurements, for example with CH, C_2, CN, NO and OH, all report sensitivities down to a few ppm. Even CH_3 can be measured in flames at levels of 65-70 ppm. The fact that under saturation conditions, DFWM intensities fall off as the square of the concentration indicates the severity of these differences. On the other hand, the degree of theoretical understanding now is quite sound for DFWM, and the levels of approximation involved would not appear to conceivably introduce the magnitude of change that is required to bring this body of data together. The DFWM spectroscopy involved, per se, appears to be reasonable and valid. An indirect calibration method, however, is used to scale the S_2 intensities and has never been validated. One plausible explanation that is proposed herein relates to the very efficient collision free coupling that occurs between the $S_2(B^3\Sigma_u^-)$ and $S_2(B''^3\Pi_u)$ states. There is evidence in the literature that the latter long-lived state can act as a pseudo-metastable state. Instantaneous depletion of the pumped $S_2(X^3\Sigma_g^-, v=2)$ into this state would modify the data by lowering the resultant values. If correct, this appears to be the first such reported interference with DFWM monitoring.

A review of the current status of our understanding of the behavior of the major sulfur species in flames indicates that any possible need for modification should be only minor. Major remaining uncertainties, which cannot noticeably perturb the sulfur chemistry itself, center on the exact nature of the mechanisms by which sulfur modifies NO_x formation and, to a lesser extent, to reexamine the validity of the exact mechanisms involved in the catalytic flame radical recombination cycles. Definitive studies of these have yet to be done.

LASER INDUCED FLUORESCENCE SPECTROSCOPY OF tert-PENTOXY AND 3-PENTOXY RADICALS

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New fluorescence excitation spectra of *tert*-pentoxy ($(CH_3)_2C(O)CH_2CH_3$) and 3-pentoxy radicals were observed in the wavelength range 345-400 nm. The radicals were produced by laser photolysis of the corresponding pentyl nitrites at 355 nm. For *tert*-pentoxy, 12 vibronic bands were labeled in three progressions, with ν_{CO}=551 cm^{-1}. The transition origin was tentatively assigned at 25491 cm^{-1} (392.3 nm). For 3-pentoxy, 9 vibronic bands were assigned to three progressions, including a with ν_{CO} of 573 cm^{-1}. The transition origin was assigned at 26439 cm^{-1} (378.2 nm). Numerous peaks in both spectra remain unassigned. The fluorescence lifetime of 3-pentoxy was determined to be about 160 ns.

EXPERIMENTAL STUDIES OF THE NaK(3^1P AND 1^3D) STATES

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We report the results of optical-optical double resonance experiments designed to study the $3^1\Pi$ and $1^3\Delta$ states of NaK. In the first step, a narrow band cw dye laser (PUMP) was tuned to excite a particular $2(A)^1\Sigma^+(v_A, J')$ level [or $2(A)^1\Sigma^+(v_A, J') \sim 1(b)^3\Pi(v_b, J')$ mixed level], and its frequency was then fixed. A second narrow band tunable cw Ti:Sapphire laser (PROBE) was then scanned over transitions to various $3^1\Pi(v_\Pi, J)$ [or $1^3\Delta(v_\Delta, J)$] levels while $3^1\Pi \rightarrow 1(X)^1\Sigma^+$ violet fluorescence [or collision-induced $^3\Lambda \rightarrow 1(a)^3\Sigma^+$ green fluorescence] was monitored. The Doppler-free signals accurately map the $3^1\Pi$ and $1^3\Delta$ state rovibrational energy levels. These energy levels were then fit to Dunham expansions to provide experimental molecular constants, allowing the construction of RKR potential curves that have been compared to recent theoretical calculations. Comparison between observed and calculated Franck Condon factors was used to determine variation of the $3^1\Pi \rightarrow 1(X)^1\Sigma^+$ transition dipole moment with internuclear separation. A deperturbation analysis of the $1^3\Delta$ state was performed to determine the spin-orbit constant for that state. The $1^3\Delta$ state hyperfine structure, due to the Fermi contact interaction between the electron spin and the sodium atom nuclear spin, was also studied.

OBSERVATION OF Na_2 GERADE LEVELS DISSOCIATING TO THE (3P+3P) ATOMIC LIMIT BY TWO-COLOR PHOTOASSOCIATION SPECTROSCOPY

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(Presented at the *Division of Atomic, Molecular and Optical Physics 2000 Meeting of the American Physical Society*, Held in Storrs CT, June 2000).

We have performed photoassociation spectroscopy of ultracold (T<1 mK) sodium atoms confined to a magneto-optical trap. With this technique, we have probed with high resolution the weakly bound vibrational levels of the $Na_2(A^1\Sigma_u^+)$ state and previously unseen $^3\Sigma_{1g}$ and $^3\Sigma_{0g-}$ states, which dissociate to the $(3S+3P_{1/2})$ atomic limit. Also, by starting in those long range states with outer turning points of 30-50 a_O, we have used a second laser to measure weakly bound levels near the (3P+3P) asymptotes which undergo associative ionization. In particular, starting from the $A^1\Sigma^+$ state, we are able to access previously unrecorded gerade levels. The signals are especially strong for levels bound by less than 2 cm^{-1} below the $(3P_{3/2}+3P_{1/2})$ asymptote.

OSCILLATOR STRENGTHS FOR (B-X, C-X AND E-X) TRANSITIONS IN CARBON MONOXIDE

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Oscillator strengths for transitions in CO were obtained at the Synchrotron Radiation Center of the University of Wisconsin-Madison. Our focus was on transitions that will be observed in interstellar spectra with the Far Ultraviolet Spectroscopic Explorer; these transitions are also important in studies of selective isotope photodissociation where fractionation among isotopomers can occur. Absorption from the ground state ($X^1\Sigma^+$ $v''=0$) to $B^1\Sigma^+(v'=0,1)$, $C^1\Sigma^+(v'=0,1)$ and $E^1\Pi(v'=0,1)$ was measured with the 4 m Normal Incidence Monochromator. The instrumental resolution was approximately 0.01 nm. As in our earlier experiment, fits to the (A-X)(5,0) band, whose oscillator strength is well known, yielded the necessary column density and excitation temperature. These parameters were used in the least-squares fit of the transitions of interest to extract their band oscillator strengths. The results will be compared with other recent determinations.

LINE OSCILLATOR STRENGTH MEASUREMENTS IN THE (0-0) BAND OF THE (c'_4-X) TRANSITION OF N_2

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Oscillator strengths for 48 rotational lines in the 0-0 band of the (c'_4-X) system of N_2, a prominent feature in planetary airglow emissions, were determined from vacuum ultraviolet photoabsorption spectra recorded with an instrumental resolution of 6.5×10^{-4} nm. Our results are compared with earlier measurements of band-integrated absorption cross sections and with a study of electron-impact-induced emission from $c'_4(0)$, as well as with electron scattering measurements and a nonadiabatic calculation of vibronic band strengths. Relative P- and R-branch absorption intensities deviate systematically from those of an unperturbed ($^1\Sigma$-$^1\Sigma$) band, as expected from the interactions of the $c'_4(v=0)$ level with nearby Rydberg and valence states. In addition, band f-values derived from pairs of R- and P-branch transitions with a common lower-state rotational level, f(J″), are found to be J-dependent. This J-dependence is discussed in the context of the interference patterns which characterize the absorption strengths in the region of the widespread interactions between Rydberg and valence state levels.

THE STRUCTURE OF O_3-CH_4 AND IMPLICATIONS FOR THE $O+CH_4$ PRECURSOR-LIMITED REACTION
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The rotational spectrum of the O_3-CH_4 complex has been measured in a molecular beam using a pulsed-nozzle Fourier-transform microwave spectrometer. An *a*-type pure-rotation and a *c*-type rotation-inversion electric-dipole spectrum is observed, complicated by the nearly free internal rotation of the CH_4 top and the inversion tunneling of the O_3. The nuclear-spin statistics of the equivalent oxygen nuclei leads to only one tunneling component existing for each rotation-internal-rotation state, indicating that the transition state has a heavy-atom. C_{2v}-symmetry geometry. The tunneling splitting is determined to be 30 to 40 MHz, dependent on the CH_4 internal-rotor state. Only two of the three methane internal-rotor states have been assigned. These two states of A and F symmetry have asymmetric-rotor energy-level structures, weakly perturbed by the ozone-inversion tunneling. Transitions have been observed for the E internal-rotor state, verified by their linear frequency shifts with electric field, however no definitive rotational assignment of these lines could be made. The E internal-rotor-state energy-level structure is complicated by the unquenched internal-rotation angular momentum of the methane top, which leads to a strong Coriolis interaction between the rotation and internal-rotation angular momenta. The zero-point structure of the complex has a heavy-atom plane of symmetry with the two terminal O atoms equidistant above and below this plane. The angle between the line joining the center of masses of the two subunits and the O_3, C_2 axis is 118.2(5)° (with the planar O directed away from the CH_4). The shortest O-C separation is 3.57. The geometry of the complex suggests two outcomes for the reaction of the O atom produced by 267 nm photolysis of O_3 in the complex, either nonreaction or reaction by stripping of a hydrogen atom at high impact parameters, leading to fast, highly rotationally excited OH product.

DIRECT, PRESSURE-DEPENDENT MEASUREMENTS OF OH AND H YIELDS FROM THE GAS PHASE REACTION OF OZONE WITH ALKENES
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The reaction of ozone with unsaturated hydrocarbons in the gas phase is believed to be an important source of HO_x radicals in the troposphere. However, since the reaction mechanism involves vibrationally excited intermediate species, and most yield measurements are indirect, the exact mechanism and product branching ratios remain uncertain. We present direct pressure-dependent measurements of radical yields for a number of ozone-alkene reactions. OH and H radicals are detected using laser induced fluorescence and resonance fluorescence, and are measured at steady state, formed from the ozone-alkene reaction and lost to reaction with the alkene. Short reaction times (usually 10 ms) ensure minimal interference from secondary reactions. Measurements from 1 torr to hundreds of torr cover a set of simple symmetric alkenes: ethene, trans-2-butene, 2,3-dimethyl-2-butene, 3-hexene, and 3,4-dimethyl-3-hexene. OH yields for the smaller alkenes are pressure independent and consistent with previous indirect measurements. However, yields for the larger alkenes decrease rapidly with pressure, resulting in 1 atm yields significantly lower than current recommendations. This pressure dependence is caused by the large number of nonreactive modes of the carbonyl oxide (Criegee) intermediate. Larger intermediates have longer lifetimes with respect to unimolecular reaction and therefore are more susceptible to collisional stabilization; we motivate this effect more quantitatively using statistical theory. Therefore, radicals are produced directly in the ozone-alkene reaction, but yields measured in environmental chambers may be overestimates due to interference by secondary reactions.

COMPUTATIONAL STUDIES OF OH RADICAL GENERATION FROM ALKENE OZONOLYSIS

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The gas phase ozonolysis of alkenes generates hydroxyl radical, and therefore can have a critical impact on tropospheric chemistry. We have explored the variation of OH yields with alkene structure using density functional theory (B3LYP/6-31G(d,p)) calculations. The ability of internal alkenes and cycloalkenes to generate OH radicals can be rationalized in terms of the Criegee mechanism. The yield of OH from these systems is controlled by the concerted cycloreversion of the primary ozonide. However, the yields of OH from ethylene and propene has been found experimentally to vary with total pressure. Our B3LYP calculations indicate that the gas phase ozonolysis of these species proceeds by diradical pathways.

KINETICS AND BRANCHING RATIO MEASUREMENTS FOR THE $C_2H_5O_2$ + NO REACTION

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The temperature dependence of the overall rate constant for the $C_2H_5O_2 + NO$ reaction and the rate constant for the minor branching channel resulting in the production of $C_2H_5ONO_2$ has been measured using the turbulent flow technique with high pressure chemical ionization mass spectrometry for the detection of reactants and products. The temperature dependence of the overall rate constant for the $C_2H_5O_2 + NO$ reaction was investigated between 299 and 213 K at 100 torr pressure, and was found to agree well with the current recommendation for atmospheric modeling. The minor reaction channel $C_2H_5O_2 + NO \rightarrow C_2H_5ONO_2$ was directly observed for the first time, and the temperature dependence of the rate constant for this channel was investigated between 298 and 213 K at 100 torr pressure. The Arrhenius expressions for the overall rate and the $C_2H_5ONO_2$ producing channel indicate a branching ratio of about 0.005 at 298 K and 0.02 at 213 K at 100 torr.

RATES OF REACTION FOR CYCLOPROPANE AND CHF_2OCHF_2(HFOC-134) WITH OH RADICALS

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Rates, temperature dependences and Arrhenius A-factors were determined for the rates of reaction of cyclopropane and CHF_2OCHF_2(HFOC-134) with hydroxyl radicals. The rates were determined by a relative method to minimize errors from trace impurities and adsorption on the walls of the reaction vessel. CF_3CHF_2(FC-125) was used as the reference for HFOC-134 rate determinations. Cyclopropane rate measurements used ethane and CHF_2CH_3(FC-152a) as references. Both compounds were measured by a stopped-flow method employing GC/MS for the detection system. Photolysis of water by means of a low pressure mercury lamp produced the hydroxyl radicals.

AB INITIO STUDY OF THE KINETICS OF THE REACTIONS OF ClO RADICALS WITH CH_xCl_{4-x}(x=1-4) OVER THE TEMPERATURE RANGE 200-2500 K

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Combustion and thermal oxidation mechanisms can become complicated as the number of elements beyond C, H and O increases, especially if halogen atoms are also present. For many of the reactions involving these species, there is little or no information regarding the kinetics and/or mechanisms of the elementary steps at high temperatures.

Model development of thermal degradation processes of chlorinated compounds in methane flames requires the knowledge of the kinetics and thermodynamics characterizing the reactions between chlorine oxide (ClO) and halomethanes.

The goal of this study is the computation of the reaction enthalpies as well as the rate constants as a function of temperature in order to shed some light in the understanding of the reactivity trends experimentally observed in the following series of reactions: $ClO + CH_xCl_{4-x} = Products (x = 1\text{-}4)$.

DEPLETION KINETICS OF CHROMIUM ATOMS BY SULFUR DIOXIDE

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The gas phase depletion kinetics of $Cr(a^7S_3, a^5S_2, a^5D_J)$ in the presence of SO_2 are reported. Chromium atoms were produced by the 248 nm photodissociation of chromium carbonyl and were detected by laser induced fluorescence. The ground state of Cr was found to react rapidly via a termolecular mechanism with sulfur dioxide. Over the temperature range 296-534 K, the limiting low pressure third-order rate constants are on the order of 10^{-28} cm^6 $molecule^{-2}$ s^{-1}, and they decrease with increasing temperature. The limiting high pressure second-order rate constants are on the order of the collision rate. The excited states deplete at rates greater than or equal to the collision rate in the presence of sulfur dioxide. Results are interpreted in terms of an electron transfer mechanism and the orbital occupancies of the Cr atomic states.

MEASUREMENTS OF THE COLLISION ENERGY DEPENDENCE OF THE $H+D_2$®$HD(n=0,j=7)+D$ REACTION

N. Shaferray and L.J. Asinghe, The University of Oklahoma (Presented at the *Division of Atomic, Molecular and Optical Physics 2000 Meeting of the American Physical Society*, Held in Storrs CT, June 2000).

The $H+H_2$ reaction and its isotopic analogs have long served as models for quantum theories of reactive scattering. Despite the importance of these reactions, surprisingly few systematic studies of their energy dependence have been carried out. Here we present measurements of the collision-energy dependence of the $H+D_2 \rightarrow HD(v=0,j=7)+D$ reaction and compare our observations with predictions of Brian Kendrick of Los Alamos National Laboratory.

MECHANISTIC STUDY OF THE REACTION OF HYDROXYL RADICALS WITH NITRIC ACID: ISOTOPICALLY SUBSTITUTED REACTIONS, PRODUCT YIELDS AND COMPARISON TO THEORY

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The reaction of hydroxyl radicals with nitric acid is one of the major pathways for generation of NO_x from HNO_3 in the atmosphere. The rate constant has an unusual pressure and temperature dependence that suggests the formation of a reactive complex. We investigate the rate constants for isotopically substituted reactants, $OD+DNO_3$, $OH+DNO_3$, $OD+HNO_3$ and $^{18}OH+HNO_3$. Deuterium substitution on nitric acid results in more than a tenfold reduction in the rate constant, while deuterium substitution on hydroxyl increases the rate constant slightly. There is no evidence for exchange in the isotopically mixed reactions. Product yield studies show that the title reaction produces nitrate radical with unit efficiency over all temperatures and pressures studied. Finally, ab initio calculations of possible reactive complex structures and their corresponding transition states corroborate the experimental observations.

HIGH RESOLUTION PHOTOFRAGMENT TRANSLATIONAL SPECTROSCOPY WITH VIBRATIONAL QUANTUM STATE RESOLUTION: PHOTODISSOCIATION OF CH_3I AT 266 nm

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A high resolution photofragment translational spectroscopy technique that enables direct resolution of vibrational quantum states has been developed and used to study the well-known model system, the photodissociation of CH_3I at 266 nm. The high resolution translational spectrum of $I(^2P_{1/2})$ fragments reveals a sole progression of the $\nu_2(a'')$ umbrella bending vibration. Vibrational state distribution of CH_3 in the I*-channel was determined to be $\nu_2=0:1:2=0.65(\pm0.02):0.29(\pm0.01):0.06(\pm0.01)$ with values of the recoil anisotropy being $1.92(\pm0.03)$, $1.87(\pm0.05)$, and $1.75(\pm0.09)$, respectively. The rotational temperature of the $\nu_2=1$ state (120 ± 40 K) was observed to be similar to that of the $\nu_2=0$ state (120 ± 30 K) reported previously. The bond dissociation energy was determined to be $D_0°(CH_3\text{-}I)=55.9(\pm0.5)$ kcal/mol. Detailed aspects of the vibrational and rotational energy partitioning as well as the recoil anisotropy are compared with the recent theoretical predictions.

ULTRAVIOLET PHOTODISSOCIATION OF NCO: WAVELENGTH DEPENDENCE OF BRANCHING AMONG PRODUCT CHANNELS

S. Gomez, H.M. Lambert and P.L. Houston, Department of Chemistry and Chemical Biology, Cornell University, Baker Laboratory, Ithaca, NY 14853-1301, Fax (607) 255-8549, sg55@cornell.edu (Presented at the *219th National Meeting of the American Chemical Society*, Held in San Francisco CA, March 2000).

The photodissociation dynamics of the NCO radical have been studied using standard pump-probe techniques. NCO is generated from the reaction of $CN + O_2$, where the CN is produced by 193 nm photolysis of C_2N_2 at the exit of a pulsed nozzle. An ultraviolet laser is tuned to a rovibrational resonance in the $B(^2\Pi) \leftarrow X(^2\Pi)$ transition, which predissociates to products, N + CO. CO products from either the $CN + O_2$ reaction or the photodissociation of NCO can be detected by sub-Doppler VUV LIF on the $A(^1\Pi) \leftarrow X(^1\sigma^+)$ transition. The CO rotational distribution and Doppler profiles provide information about the branching between dissociation to coproducts: $N(^4S)$, $N(^2D)$ and $N(^2P)$. Recent results will be presented.

UNIMOLECULAR REACTION DYNAMICS OF VINYL CHLORIDE ON THE GROUND ELECTRONIC POTENTIAL ENERGY SURFACE: EXCITATION BY CHEMICAL ACTIVATION AND PRODUCT STATE DISTRIBUTIONS OF HCl AND Cl FRAGMENTS

Y.S. Choi, S.K. Kim, S.H. Cho, W.-H. Park and S.-M. Lim, Department of Chemistry, Inha University, Nam-gu, Incheon, 402-751, South Korea, Fax (82) 32-867-5604, yschoi@inha.ac.kr (Presented at the *219th National Meeting of the American Chemical Society*, Held in San Francisco CA, March 2000).

The dynamics of unimolecular reactions of vinyl chloride on the ground electronic potential energy surface have been investigated. The vibrationally excited vinyl chloride in its ground electronic state was prepared by using the isomerization of methyl-chlorocarbene radical to vinyl chloride via H-atom migration and the carbene radicals were produced by photolysis of 3-methyl-3-chlorodiazirine at 353.6 nm. The vinyl chloride molecules formed in this excitation scheme were highly vibrationally excited in its ground electronic state due to the bond formation between two carbon atoms, and were found to undergo unimolecular reactions of HCl elimination and C-Cl bond fission. The rotational and vibrational energy distribution of HCl fragments and the spin-orbit state branching ratio of Cl atoms have been measured with resonantly enhanced multiphoton ionization (REMPI)/time-of-flight mass spectrometry. The overall state distribution of HCl and Cl fragments are much colder than those of 193 nm photodissociation as expected from the smaller excitation energy. Interestingly, however, the rotational distribution of HCl(v=0) fragments fits to a Boltzmann distribution of a single rotational temperature in contrast to the result of 193 nm photodissociation, which showed a bi-exponential distribution. The dynamical differences between two excitation schemes will be discussed in terms of the potential energy surfaces involved.

NONADIABATIC TRAJECTORIES AT AN EXHIBITION

M.D. Hack and D.G. Truhlar, Department of Chemistry and Supercomputer Institute, University of Minnesota, Minneapolis, MN 55455 (to Appear in the *Journal of Physical Chemistry A.*).

The present article reviews two classes of semiclassical (mixed quantum mechanical/classical) methods for investigating multi-electronic-state dynamics: the trajectory surface hopping (TSH) method and the time-dependent self-consistent field (TDSCF) method. The recent availability of accurate quantum mechanical dynamics calculations for a variety of realistic three-body two-state potential energy matrices has allowed an assessment of the validity of semiclassical multi-surface dynamics methods that are applicable to larger systems. These studies indicate that Tully's fewest switches algorithm is the best available TSH method and that the Ehrenfest method is the best previously available TDSCF method. The fewest switches surface hopping

method has relatively small errors even when it is not the best method, while the Ehrenfest TDSCF method tends to have larger errors when it is not the best. However, the fewest switches algorithm involves unphysical discontinuities in momenta and the results may depend on the choice of representation. Furthermore, the surface hopping algorithm is frequently frustrated in its attempt to maintain ensemble-average self consistency. The Ehrenfest method removes all these troublesome aspects but at the cost of producing unphysical mixed states which are responsible for its larger errors in observables. A recently introduced TDSCF method, the continuous surface-switching method, removes the unphysical mixed states of the Ehrenfest method, and in initial tests it produces results that are systematically better than those calculated by the Ehrenfest method. The present article illustrates several of these aspects of nonadiabatic trajectory methods pictorially.

CONTINUOUS SURFACE SWITCHING: AN IMPROVED TIME-DEPENDENT SELF-CONSISTENT-FIELD METHOD FOR NONADIABATIC DYNAMICS

Y.L. Volobuev, M.D. Hack, M.S. Topaler and D.G. Truhlar, Department of Chemistry and Supercomputer Institute, University of Minnesota, Minneapolis, MN 55455 (to Appear in the *Journal of Chemical Physics*).

We present a new semiclassical method for electronically nonadiabatic collisions. The method is a variant of the time-dependent self-consistent field method and is called continuous surface switching. The algorithm involves a self-consistent-potential trajectory-surface-switching approach that is designed to combine the advantages of the trajectory-surface-hopping approach and the Ehrenfest classical-path self-consistent-potential approach without their relative disadvantages. Viewed from the self-consistent perspective, it corresponds to "on-the-fly histogramming" of the Ehrenfest method by a natural decay of mixing; viewed from the surface hopping perspective, it corresponds to replacing discontinuous surface hops by continuous surface switching. In this paper we present the method and illustrate it for three multidimensional cases. Accurate quantum mechanical scattering calculations are carried out for these three cases by a linear algebraic variational method, and the accurate values of reactive probabilities, quenching probabilities, and moments of final vibrational and rotational distributions are compared to the results of continuous surface switching, the trajectory-surface-hopping method in two representations, the time-dependent self-consistent-field method, and the Miller-Meyer classical electron method to place the results of the semiclassical methods in perspective.

USE OF AB INITIO QUANTUM MECHANICS TO ESTIMATE RATE CONSTANTS

D.M. Golden, Department of Mechanical Engineering, Stanford University & SRI International, Stanford, CA 94305, Fax (650) 859-6196, golden@sri.com, and J.P. Senosiain and C.B. Musgrave, Department of Chemical Engineering, Stanford University (Presented at the *219th National Meeting of the American Chemical Society*, Held in San Francisco CA, March 2000).

Understanding complex chemical systems, such as the chemistry of the polluted urban atmosphere, require a mathematical model describing the physics and chemistry of the assemblage. Despite many years of laboratory experiments that have improved our understanding immensely, it is not possible to measure every possible reaction that should be considered in the model. Thus, estimation techniques based on laboratory understanding have been used extensively. Often, however, insufficient experimental measurements exist with which to begin extrapolation of larger molecules. Recent advances in computational quantum mechanics have made it possible to compute potential energy surfaces for reactions that have not been measured. It would then seem possible to compute gas phase rate constants from judicious use of transition state theory (TST) and/or the microcanonical version applied to unimolecular reactions and their reverse known as RRKM theory. We have set out to test this posit by computing the structural properties of reactants

and transition states needed to apply the above theory. We have computed these properties for the reaction X+ethane=HX+ethyl for X=H, O, OH, NH_2, CH_3 and Cl. The thermochemistry is well-known for these reactions and the rate constants have been measured as functions of temperature for all of them. We have employed the following quantum chemistry methods: B3LYP, MP2 and QCISD and used the gaussian basis sets: 6-311G(d,p) and 6-311++G(3df,2dp). We first examined the computed values for ΔH for the reaction. As has been noted by others, the structures and frequencies for the stable molecules and the transition states were similar for all levels of calculation. Thus we used the B3LYP structures and frequencies in conjunction with a TST code that compares experimental rate constants as functions of temperature with computed values, accepting the B3LYP structural information for reactants and transition states, while searching for the best value of the activation barrier (ΔH_0). (Tunneling is accounted for iteratively using Eckart corrections.) We have found that using the ab initio structures we cannot fit the Arrhenius curvature measured for either OH or NH_2 with ethane.

ADIABATIC CONNECTION FOR KINETICS

B.J. Lynch, P.L. Fast, M. Harris and D.G. Truhlar, Department of Chemistry and Supercomputer Institute, University of Minnesota, Minneapolis, MN 55455 (to Appear as a Letter in the *Journal of Physical Chemistry A*.).

A new hybrid Hartree-Fock-density functional (HF-DF) model called the modified Perdew-Wang 1-parameter model for kinetics (MPWIK) is optimized against a database of 20 forward barrier heights, 20 reverse barrier heights, and 20 energies of reaction. The results are compared to other hybrid HF-DF methods with the 6-31+G(d,p) basis. The new method reduces the mean unsigned error in reaction barrier heights by a factor of 2.4 over MPW1PW91 and by a factor of 3 over B3LYP.

ADDITION REACTION OF PROPARGYL AND ACETYLENE

N.W. Moriarty and M. Frenklach, Department of Mechanical Engineering, University of California, Berkeley, CA 94720, Fax (510) 642-1850, moriarty@me.berkeley.edu, X. Krokidis, French Institute of Petroleum, and W.A. Lester, Department of Chemistry, University of California (Presented at the *219th National Meeting of the American Chemical Society*, Held in San Francisco CA, March 2000).

The addition of acetylene and propargyl has been investigated using several DFT methods including B3-LYP, B3-PW91 and B&H-H&LYP. The optimized geometries were calculated using the 6-31G(d,p) and the cc-pVTZ basis sets. Quantum Monte Carlo calculations were performed at the B3-LYP/cc-pVTZ optimized geometries. The RRKM rate constants were determined for the reactions leading to the formation of the *c*-C_5H_5 radical. The heat of formation and rate of decomposition of the radical are determined and compared with experiment. A detailed analysis of the reaction pathways is performed using the Bonding Evolution Theory concepts applied to the Electron Localization Function.

QUANTUM DYNAMICS OF HOCl MOLECULE ON ACCURATE POTENTIAL ENERGY SURFACE

S. Skokov and J.M. Bowman, Department of Chemistry, Emory University, 1515 Pierce Drive, Atlanta, GA 30322, Fax (404) 727-6628, skokov@euch3g.chem.emory.edu, and K.A. Peterson, Department of Chemistry, Washington State University, Richland, WA 99352 (Presented at the *219th National Meeting of the American Chemical Society*, Held in San Francisco CA, March 2000).

Accurate ab initio multireference CI calculations with large correlation-consistent basis sets have been performed for HOCl. After extrapolation to the complete basis set limit the ab initio data have been precisely fit to give a global three-dimensional potential energy surface. The surface was corrected by inverse perturbation method to reproduce exactly experimental vibrational energies and rotational constants. Variational calculations were performed for

rovibrational bound states of HOCl and HClO isomer. Rotation induced Fermi coupling is analyzed and compared to available experimental data. Complex L2 calculations are carried out for resonance rovibrational states of HOCl, within adiabatic rotation approximation, and compared to experimental data. The variation of state-selected dissociation rates is shown to be due to rotation induced coupling. The importance of isotope effect and coriolis coupling on the dissociation rate is discussed. We also report preliminary results on quantum reactive scattering for $O(^1D)+HCl$ reaction.

ATMOSPHERIC ABSORPTION OF Nd:YAG LASER RADIATION

W. Butler, S. Bentley, R. Boyd and A. Melissinos, University of Rochester (Abstract Presented at the *April Meeting 2000 of the American Physical Society*, Held in Long Beach CA, April 2000).

We have measured the absorption coefficient of infrared radiation at 1064 nm in air as a function of the partial pressure of the water vapor content. We used an NPRO laser locked to a Fabry-Perot cavity of high finesse F=12,000 filled with air. The incident power was $P_0 \cong 500$ mW and the build-up factor 1314 leading to a stored power $P_S \cong 660$ W. We recorded the change in frequency $\Delta\nu/\nu$ (by using a second lower finesse F-P) and thus the local change in temperature ΔT, as a function of the stored power P_S. This allows us to determine α/κ where α is the absorption coefficient and κ the thermal conductivity of air for which we use $\kappa = 0.24 \times 10^{-3}$ W/cm-K. We then find that at about 20 °C and relative humidity 24%, α/κ varies linearly with pressure and $\alpha = 8(\pm 2) \times 10^{-9}$ (P/1 atm)cm^{-1}. This result is within the range of model calculations, but our measurements indicate that α is independent or the relative humidity.

DIABATIC AND ADIABATIC POTENTIAL CURVES FOR OH^+, AND CHARGE EXCHANGE CROSS SECTIONS FOR $O+H^+ \leftrightarrow O^++H$

A.P. Hickman, and J.A. Spirko, Lehigh University (Presented at the *Division of Atomic, Molecular and Optical Physics 2000 Meeting of the American Physical Society*, Held in Storrs CT, June 2000).

We have implemented large scale electronic structure calculations of diabatic and adiabatic potential curves for several $^3\Sigma^-$ states of OH^+. The methodology is an implementation of the CAS-SCF-CI method followed by block diagonalization, following Domcke and co-workers and Pacher et al. The potentials calculated are needed for coupled channel calculations for the charge exchange of H^+ with O (and the reverse process). This scattering process is of great importance in the upper atmosphere and in interstellar space. A key feature of the analysis is the near degeneracy (within 1 cm^{-1}) of the asymptotic fine structure levels $O(^3P_1)+H^+$ and $O^+(^4S)+H$. The diabatic potential curves are well suited to such a situation, because the asymptotic limits of the diagonal elements can be adjusted to match spectroscopic values. Adiabatic and diabatic potential curves and the current state of the calculations will be presented at the meeting.

MC-QCISD: MULTI-COEFFICIENT CORRELATION METHOD BASED ON QUADRATIC CONFIGURATION INTERACTION WITH SINGLE AND DOUBLE EXCITATIONS

P.L. Fast and D.G. Truhlar, Department of Chemistry and Supercomputer Institute, University of Minnesota, Minneapolis, MN 55455 (to Appear in the *Journal of Physical Chemistry A.).*

This paper presents a multi-coefficient correlation method based on quadratic configuration interaction with single and double excitations (MC-QCISD) and basis sets using segmented contraction and having the same exponential parameters in the s and p spaces. The results are comparable to a previous multi-coefficient correlation method based on coupled cluster theory with less efficient correlation-consistent basis sets, and they are better than a previous multi-coefficient correlation method based on Moller-Plesset fourth order perturbation theory with single, double, and quadruple excitations with correlation-consistent basis functions. The mean

unsigned error per bond of the MC-QCISD method is 0.74 kcal/mol. The new method should be very efficient for computing geometries of open-shell transition states.

HEAT OF FORMATION OF OBrO: AN EXPERIMENTAL PHOTOIONIZATION STUDY

R.B. Klemm, Department of Applied Science, Brookhaven National Laboratory, P.O. Box 5000, Upton, NY 11973, Fax (516) 344-7905, klemm@bnl.gov, R.P. Thorn and L.J. Stief, NASA/Goddard Space Flight Center, Greenbelt, MD 20771, and T.J. Buckley, Physical and Chemical Properties Division, National Institute of Standards and Technology, Gaithersburg, MD 20899 (Presented at the *219th National Meeting of the American Chemical Society*, Held in San Francisco CA, March 2000).

The potential importance of OBrO in atmospheric chemistry has been suggested recently. Although there appear to be no experimental measurements of $\Delta H(OBrO)$, estimated values range from 70 to 152 kJ/mol [Chase, *J. Phys.Chem. Ref. Data* 25, 1069, 1297 (1996)]. In the present investigation, the appearance energy (AE) or BrO^+ from OBrO was measured by employing a discharge flow-photoionization mass spectrometer that is operated at beamline U-11 (National Synchrotron Light Source/Brookhaven National Lab). The heat of formation was derived from the AE result and the ionization energy of OBrO [IE=10.29 eV, Thorn et al., *J. Phys. Chem. A.* 103, 8384 (1999)]. The AE experiments yield a threshold at about 98.7 nm that gives, in turn, a value for $\Delta H(OBrO)$ of 180($\pm$10) kJ/mol. The difference with the estimated values mentioned above and the concomitant implications for the atmospheric reactions of OBrO will be discussed.

TECHNICAL MEETINGS

(Current Additions to this List are Indicated by a Diamond Bullet Marking)

JULY 30-AUGUST 4, 2000

SPIE ANNUAL MEETING
San Diego CA.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

JULY 30-AUGUST 4, 2000

28th INTERNATIONAL SYMPOSIUM ON COMBUSTION
Edinburgh, Scotland.

Information: S.S. Terpack, The Combustion Institute, 5001 Baum Boulevard, Suite 635, Pittsburgh, PA 15212, (412) 687-1366, Fax (412) 687-0340, e-mail: combust@telerama.lm.com

JULY 30-AUGUST 4, 2000

GORDON RESEARCH CONFERENCE ON MOLECULAR ELECTRONIC SPECTROSCOPY AND DYNAMICS
New London NH.

Information: R.W. Field, Chair, Massachusetts Institute of Technology, rwfield@mit.edu; E. Bernstein, Vice-chair, Colorado State University, erb@lamar.colostate.edu; or J. Skinner, Chair, University of Wisconsin-Madison, skinner@chem.wisc.edu

AUGUST 6-11, 2000

15th INTERNATIONAL CONFERENCE ON NUCLEATION AND ATMOSPHERIC AEROSOLS
Rolla MO.

Information: B. Hale, University of Missouri, 205 Physics, Rolla, MO 65409, (573) 341-4795, e-mail: bhale@umr.edu or marrku.kulmala@helsinki.fi, http://www.umr.edu/~icnaa

AUGUST 6-11, 2000

16th IUPAC CONFERENCE ON CHEMICAL THERMODYNAMICS
Halifax, Nova Scotia, Canada.

Information: M.A. White, Department of Chemistry, Dalhousie University, Halifax, Nova Scotia B3H 4J3, Canada, (902) 494-3894, Fax (902) 494-1310, e-mail: mary.anne.white@dal.ca, http://IS.DAL.CA/~ICCT

AUGUST 8-12, 2000

8th INTERNATIONAL CONFERENCE ON ELECTRONIC SPECTROSCOPY AND STRUCTURE
Berkeley CA.

Information: ICESS8, Advanced Light Source, Lawrence Berkeley National Laboratory, MS 6-2100, Berkeley, CA 94720, Fax (510) 486-4773, e-mail: icess@lbl.gov, http://www-als.lbl.gov/icess

AUGUST 13-16, 2000

5th INTERNATIONAL CONFERENCE ON GREENHOUSE GAS TECHNOLOGIES
Cairns, Queensland, Australia.

Information: GHGT-5 Secretariat, C. Paulson, CSIRO Energy Technology, PO Box 136, North Ryde, NSW 1670, Australia, (2) 9490-8790, Fax (2) 9490-8819, e-mail: c.paulson@det.csiro.au

AUGUST 13-18, 2000

TURBINE 2000, INTERNATIONAL SYMPOSIUM ON HEAT TRANSFER IN GAS TURBINE SYSTEMS
Izmir, Turkey.

Information: R.J. Goldstein, Conference Chair, Department of Mechanical Engineering, University of Minnesota, Minneapolis, MN 55455, (612) 625-5552, Fax (612) 625-3434, e-mail: rjgumn@mailbox.mail.umn.edu, http://ichmt.me.metu.edu.tr
Deadline: Abstracts Due by February 29, 2000.

AUGUST 14-17, 2000

18th AIAA APPLIED AERODYNAMICS CONFERENCE
Denver CO.

Information: N.E. Suhs, Applied Aerodynamic Technical Program Chair, Naval Air Systems Command, Building 2187, Unit 5, Suite 1390A, 48110 Shaw Road, Patuxent River, MD 20670, (301) 342-0311, Fax (301) 342-8585, e-mail: suhsne@navair.navy.mil, or http://www.aiaa.org/calendar
Deadline: Abstract by January 3, 2000

AUGUST 14-18, 2000

12th INTERNATIONAL CONGRESS ON THERMAL ANALYSIS AND CALORIMETRY
Copenhagen, Denmark.

Information: O.T. Sorensen, Materials Research Department, Riso National Laboratory, DK-4000 Roskilde, Denmark, 45-4677-5800, Fax 45-4677-5758, e-mail: o.toft.sorensen@risoe.dk, http://www.risoe.dk/ictac

AUGUST 16-22, 2000

JAHN TELLER SYMPOSIUM
Boston MA.

Information: M. Kaplan, Simmons College and Boston University, (617) 521-2727, e-mail: kaplan@buphy.bu.edu, or G. Zimmerman, Boston University, (617) 353-2189, e-mail: goz@buphy.bu.edu

AUGUST 20-22, 2000

34th ASME NATIONAL HEAT TRANSFER CONFERENCE
Pittsburgh PA.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7795, Fax (212) 705-7143, http://www.asme.org

AUGUST 20-24, 2000

220th NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Washington DC.

Division of Analytical Chemistry:
- Detection of Explosives, Pre- and Post-Blast
  R.Q. Thompson, Oberlin College, Department of Chemistry, 130 W. Lorain Street, Oberlin, OH 44074, (440)775-8305, Fax (440) 775-6682, e-mail: robert.q.thompson@oberlin.edu

Division of Fuel Chemistry:
- 1990 Clean Air Act Amendments: A 10-Year Assessment
  J.J. Helble, University of Connecticut, Department of Chemical Engineering, U-222, Storrs, CT 06269, (860) 486-4602, Fax (860) 486-2959, e-mail: helble@eng2.uconn.edu
- Inorganics in Fossil Fuels, Waste Materials, and Biomass: Characterization, Combustion Behavior, and Environmental Issues
  C.L. Senior, Physical Sciences, Inc., 20 New England Business Center, Andover, MA 01810, (978) 689-0003, Fax (978) 689-3232, e-mail: senior@psicorp.com
- Waste Material Recycling for Energy and Other Applications
  S.V. Pisupati, Fuel Science Program, Pennsylvania State University, 404 Academic Projects Building, University Park, PA 16802, (814) 865-0874, Fax (814) 863-8892, e-mail: sxp17@psu.edu
- Fossil Fuels and Global Climate/CO_2 Abatement
  R. Warzinski, USDOE/FETC, Box 10940, Building 83-324, Pittsburgh, PA 15236, (412) 892-5863, e-mail: warzinsk@fetc.doe.gov
- Production of Fuels and Chemicals from Synthesis Gas
  D.B. Dadyburjor, Department of Chemical Engineering, P.O. Box 6102, West Virginia University, Morgantown, WV 26506, (304) 293-2111 ext 2411, Fax (304) 293-4139, e-mail: dadyburjor@cemr.wvu.edu
- Solid Fuel Chemistry
- Chemistry of Liquid and Gaseous Fuels
  F. Huggins, South Limestone St., Suite 111, University of Kentucky, Lexington, KY 40506, (606) 257-4045, Fax (606) 257-7215, e-mail: fhuggins@engr.uky.edu
- CO_2 Capture, Utilization and Sequestration
  R.P. Warzinski, Department of Energy, Federal Energy Technology Center, P.O. Box 10940, Building 83-324, Pittsburg, PA 15236, (412) 386-5863, Fax (412) 386-4806, e-mail: warzinsk@fetc.doe.gov; R.M. Enick, University of Pittsburgh, Department of Chemical

Engineering, 323 Benedum Engineering Hall, Pittsburgh, PA 15261, (412) 624-9649, e-mail: enick@engrng.pitt.edu

- Solid Fuel Chemistry and
- Chemistry of Liquid and Gaseous Fuels
  F.E. Huggins, University of Kentucky, Chemical and Materials Engineering, 533 S. Limestone Street, 111 Whalen Building, Lexington, KY 40506, (606) 257-4045, Fax (606) 257-7215, e-mail: fhuggins@engr.uky.edu

Division of Petroleum Chemistry:

- Emission Control in Petroleum Processing
  P. O'Connor, U.S. Ozkan, Department of Chemical Engineering, Ohio State University, 140 W. 19th Avenue, Columbus, OH 43210, (614) 292-6623, Fax (614) 292-3769, e-mail: ozkan.1@osu.edu
- Structure of Jet Fuels VI
  W.E. Harrison, Department of the Air Force, WL/POSF, Building 490, Area B, 1790 Loop Road N., Wright-Patterson AFB, OH 45433, (937) 255-6601, Fax (937) 255-1125, e-mail: harriswe@wl.pafb.af.mil

Division of Physical Chemistry:

- Chemistry Under Extreme Conditions
  R. Morris, AFRL/VSBP, 29 Randolph Rd., Hanscom AFB, MA 01731, (781) 377-8758, Fax (781) 377-5088, e-mail: morris@plh.af.mil
- Very Low Temperature Spectroscopy and Dynamics
  W. Stwalley, Department of Physics, University of Connecticut, 2152 Hillside Road, Storrs, CT 06269, (860) 486-4924, Fax (860) 486-3346, e-mail: stwalley@uconnvm.uconn.edu
- Femtochemistry: Honoring Ahmed Zewail, the 1999 Chemistry Nobel Laureate
  M. Dantus, Department of Chemistry, Michigan State University, East Lansing, MI 48824-1322, (517) 355-9715, Fax (517) 353-1793, e-mail: dantus@msu.edu

Information: From the Individual Chairpersons or from the Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

AUGUST 20-25, 2000

17th INTERNATIONAL CONFERENCE ON RAMAN SPECTROSCOPY
Beijing, China.

Information: Shu-Lin Zhang, President of ICORS 2000, e-mail: icors@pku.edu.cn, http://icors.pku.edu.cn

AUGUST 22-25, 2000

9th INTERNATIONAL (MILLENNIUM) SYMPOSIUM ON FLOW VISUALIZATION
Edinburgh, Scotland.

Information: I. Grant, Heriot-Watt University, Edinburgh, Scotland, EH10 5PJ, UK, (44) 1314478800, Fax (44) 1314478660, e-mail: 9misfv@ode-web.demon.co.uk, Web Site: http://www.ode-web.demon.co.uk/9misfv
Deadline: Abstract Template should be Downloaded from the Web. 4 Pages or Less to be Submitted by December 12, 1999. Final Manuscripts Due May 15, 2000.

AUGUST 26-30, 2000

15th EUROPHYSICS CONFERENCE ON ATOMIC AND MOLECULAR PHYSICS OF IONIZED GASES
Miskolc-Lillafured, Hungary.

Information: Z. Donko, c/o Eotvos Lorand Physical Society, H-1371 Budapest, P.O. Box 433, Hungary, e-mail: escampig@elft.mtesz.hu, http://elft.mtesz.hu/escampig2000

AUGUST 27-31, 2000

14th INTERNATIONAL CONGRESS OF CHEMICAL AND PROCESS ENGINEERING
Prague, Czech Republic.

Information: CHISA 2000, Novotneho Lavka 5, 116 68 Praha 1, Czech Republic, (420) 2-2108-2333, Fax (420) 2-2108-2336, e-mail: chisa@csvts.cz, http://www.chisa.cz

AUGUST 27-SEPTEMBER 1, 2000

25th EUROPEAN CONGRESS ON MOLECULAR SPECTROSCOPY
Coimbra, Portugal.

Information: R. Fausto, Department of Chemistry, University of Coimbra, Coimbra, Portugal P-3049, (351) 39-852080, Fax (351) 39-827703, e-mail: rfausto@gemini.ci.uc.pt, http://qui.uc.pt/~rfausto/eucmos_xxv

AUGUST 27-SEPTEMBER 1, 2000

15th INTERNATIONAL MASS SPECTROMETRY CONFERENCE
Barcelona, Spain.

Information: Ana Costeja, Palau de Congressos, Departament de Convencions, Av. Reina Mª Cristina, s/n, 08004 Barcelona, Spain (34) 932-332-377, Fax (34) 934-262-845, e-mail: 15imsc@website.es, http://www.website.es/15imsc

SEPTEMBER 3-7, 2000

16th INTERNATIONAL CONFERENCE ON HIGH RESOLUTION MOLECULAR SPECTROSCOPY
Prague, Czech Republic.

Information: S. Urban, UFCH JH Academy of Sciences of the Czech Republic, Dolejskova 3, Prague, Czech Republic, CZ-18223, (420) 2-6605-3635, Fax (420) 2-858-2307, e-mail: praha2k@jh-inst.cas.cz, http://www.chem.uni-wuppertal.de/conference/

♦ SEPTEMBER 3-8, 2000

11th EUROPEAN CONFERENCE ON DIAMOND, DIAMOND-LIKE MATERIALS, CARBON NANOTUBES, NITRIDES AND SILICON CARBIDE
Porto, Portugal.

Information: L. Reed, Conference Secretariat, e-mail: e.reed@elsevier.co.uk, http://www.elsevier.nl/locate/diamondconf

SEPTEMBER 4-8, 2000

EUROPEAN AEROSOL CONFERENCE
Trinity College, Dublin, Ireland.

Information: The Aerosol Society, P.O. Box 34, Portishead, Bristol, BS20 7FE, UK, http://www.aerosol-soc.org.uk

SEPTEMBER 10-13, 2000

3rd EUROPEAN THERMAL SCIENCES CONFERENCE
Heidelberg, Germany.

Information: E. Hahne, Institut fur Thermodynamik und Warmetechnik, Pfaffenwaldring 6, 70550 Stuttgart, Germany, 49 (0) 711-685-3536, Fax 49 (0) 711-685-3503, e-mail: pm@itw.uni-stuttgart.de

SEPTEMBER 10-15, 2000

CONFERENCE ON LASERS AND ELECTRO-OPTICS (CLEO) AND THE INTERNATIONAL QUANTUM ELECTRONICS CONFERENCE (IQEC)
Nice, France.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, e-mail: confserv@osa.org

SEPTEMBER 10-15, 2000

1st INTERNATIONAL SYMPOSIUM ON MICROGRAVITY RESEARCH AND APPLICATION IN PHYSICAL SCIENCES AND BIOTECHNOLOGY
Sorrento, Italy.

Information: ESTEC, Conference Bureau, P.O. Box 299, 2200 AG Noordwijk, The Netherlands, (71) 5655005, Fax (71) 5655658, e-mail: confburo@estec.esa.nl

SEPTEMBER 10-15, 2000

7th DURHAM CONFERENCE ON PLASMA SOURCE MASS SPECTROMETRY
Durham UK.

Information: G. Holland, Department of Geological Sciences, Science Laboratories, South Road, Durham City DH1 3LE, UK, e-mail: tannersd@sciex.com, (44) 191-374-2526, Fax (44) 191-374-2510.

SEPTEMBER 12-14, 2000

3rd UNITED KINGDOM MEETING ON COAL RESEARCH AND ITS APPLICATIONS
Birmingham, UK.

Information: H.J. Graham, Power Technology Centre, Radcliffe-on-Soar, Nottingham NG11 0EE, UK, 44(0)115-936-2460, Fax 44(0)115-936-2205, e-mail: helen.graham@powertech.co.uk

SEPTEMBER 13-16, 2000

2nd INTERNATIONAL CONFERENCE ON INORGANIC MATERIALS
Santa Barbara CA.

Information: Sarah Wilkinson, Conference Secretariat, Elsevier Science Ltd., The Boulevard, Langford Lane, Kidlington, Oxford, UK OX5 1GB, 44(0) 1865 843691, Fax 44(0) 1865 843658, e-mail: sm.wilkinson@elsevier.co.uk, http://www.elsevier.com/locate/im2000

SEPTEMBER 18-20, 2000

13th INTERNATIONAL SYMPOSIUM ON GAS FLOW AND CHEMICAL LASERS AND HIGH POWER LASER CONFERENCE
Florence, Italy.

Information: C. Pescucci, Fax 39(0) 55-233-7755, e-mail: gcl-hpl@ino.it, www.ino.it/GCL-HPL or www.es.titech.ac.jp/~kkasuya/gcl-web/index.html

SEPTEMBER 19-21, 2000

THE HYDROGEN ENERGY FORUM 2000
Munich, Germany.

Information: The Future Energies Forum, "Forum fur Zukunftsenergien", Godesberger Allee 90, D-53175 Bonn, Germany, Fax 49(0) 228-959 56-50, e-mail: energie.forum@t-online.de

SEPTEMBER 22-30, 2000

27th ANNUAL CONFERENCE OF THE FEDERATION OF ANALYTICAL CHEMISTRY AND SPECTROSCOPY SOCIETIES
Nashville TN.

Information: Division of Analytical Chemistry, FACSS, (505) 820-1648, Fax (505) 989-1073, Web Site: http://FACSS.org/info.html

SEPTEMBER 23-26, 2000

ASME FALL TECHNICAL CONFERENCE OF THE INTERNAL COMBUSTION ENGINE DIVISION
Peoria IL.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7054, Fax (212) 705-7143, http://www.asme.org

SEPTEMBER 24-26, 2000

1st ROMANIAN INTERNATIONAL CONFERENCE ON ANALYTICAL CHEMISTRY
Brasov, Romania.

Information: G.L. Radu, University of Bucharest, Faculty of Chemistry, 4-12, Elisabeta Blvd., Bucharest, Romania 703461, 40(1) 220 77 80/220 79 09, Fax 40(1) 220 76 95, e-mail: lucian@ibd.dbio.ro

SEPTEMBER 29-30, 2000

FOUR CORNERS SECTION FALL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Fort Collins CO.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 2-5, 2000

ICALEO 2000, INTERNATIONAL CONFERENCE ON APPLIED LASER APPLICATIONS AND ELECTROOPTICS
Dearborn MI.

Information: E. Cohen, Laser Institute of America, (800) 345-2737 or (407) 380-1553, Fax (407) 380-5588, http://www.laserinstitute.org

OCTOBER 2-6, 2000

5th INTERNATIONAL AEROSOL SYMPOSIUM
Budapest, Hungary.

Information: N.N. Belov, Hungary, 1046 Budapest, Deak F. u., 26/a Belov N., Tel/Fax (36) 1-3791251, e-mail: belov@inext.hu, http://www.ias.inext.hu/uk-ias5-spo.htm.

♦ OCTOBER 4-5, 2000

FLAMMABLE AND COMBUSTIBLE LIQUIDS SYMPOSIUM
Baltimore MD.

Information: SFPE, 7314 Wisconsin Ave Suite, Bethesda, MD 20814, (301) 718-2910, Fax (301) 718-2242, http://www.sfpe.org/educational_programs.html

OCTOBER 8-11, 2000

GASIFICATION TECHNOLOGIES CONFERENCE
San Francisco CA.

Information: M. Samoulides, (650) 855-2127, or Electric Power Research Institute, 1412 Hillview Avenue, Palo Alto, CA 94304, (650) 855-2599, http://www.epri.com

OCTOBER 13-14, 2000

OHIO SECTION FALL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Toledo, OH.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 16-19, 2000

INTERNATIONAL FUEL AND LUBRICANTS FALL MEETING AND EXPOSITION OF THE SOCIETY OF AUTOMOTIVE ENGINEERS
Baltimore MD.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, Web Site: http://www.sae.org

OCTOBER 17-20, 2000

BEIJING INTERNATIONAL CONFERENCE ON APPLIED COMPUTATIONAL FLUID DYNAMICS
Beijing, China.

Information: Z. Tianyuan, Institute of Applied Physics and Computational Mathematics, (86) 10-62374357, Fax (86) 10-62010108, e-mail: zty@mail.iapcm.ac.cn, http://www.ciccst.org.cn/acfd

OCTOBER 19-20, 2000

SAMPLING, ON-SITE ANALYSIS AND SAMPLE PREPARATION CONFERENCE
Pittsburgh PA.

Information: B. Sherman, PACS, 409 Meade Dr., Coraopolis, PA 15108, (724) 457-6576 or (800) 367-2587, Fax (724) 457-1214, e-mail: hnpacs@aol.com, http://members.aol.com/hnpacs/pacs.htm

♦ OCTOBER 19-21, 2000

CONFERENCE ON PHOTOPHYSICS AND PHOTOCHEMISTRY
Oeiras, Portugal.

Information: A. Macanita, ITQB, AP 127, Oeiras, Portugal, 2781-901, (351) 21-4411277, e-mail: pp2000@itqb.unl.pt, http://www.itqb.unl.pt/pp2000/

♦ OCTOBER 20-21, 2000

NEW YORK SECTION FALL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Buffalo NY.

Information: M. DeMarco, Department of Physics, SUNY-Buffalo State College, 1300 Elmwood Ave., Buffalo, NY 14222, (716) 878-5230, e-mail: DemarcMJ@buffalostate.edu

OCTOBER 20-28, 2000

ANNUAL MEETING OF THE OPTICAL SOCIETY OF AMERICA AND THE INTERDISCIPLINARY LASER SCIENCE CONFERENCE
Providence RI.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, e-mail: confserv@osa.org, http://www.osa.org/mtg_conf
Deadline: Abstracts Due by May 16, 2000

OCTOBER 22-27, 2000

198th NATIONAL MEETING OF THE ELECTROCHEMICAL SOCIETY
Phoenix AZ.

Information: The Electrochemical Society, Inc., Meetings Department, 10 South Main Street, Pennington, NJ 08534, (609) 737-1902, Fax (609) 737-2743, e-mail: ecs@electrochem.org, http://www.electrochem.org/meetings/198/meet.html

OCTOBER 24-27, 2000

53rd ANNUAL GASEOUS ELECTRONICS CONFERENCE OF THE AMERICAN PHYSICAL SOCIETY
Houston TX.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 25-28, 2000

35th MIDWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
St Louis MO.

Information: C.D. Spilling, Department of Chemistry, University of Missouri, St. Louis, 80001 Natural Bridge Road, St. Louis, MO 63121 (314) 516-5313, Fax (314) 553-5342, e-mail: cspill@umsl.edu

OCTOBER 25-28, 2000

36th WESTERN REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
San Francisco CA.

Information: N.D. Byington, Customs Service Laboratory, 630 Sansome Street, Room 1429, San Francisco, CA 94111, (415) 705-4405 ext. 216, Fax (415) 705-4236, e-mail: byington@crl.com; or S. Rodriguez, Chemistry Department, University of the Pacific, Stockton, CA 95211, (209) 946-2598, Fax (209) 946-2607, e-mail: srodriguez@uop.edu

OCTOBER 28-29, 2000

JOINT FALL MEETING OF THE TEXAS SECTIONS OF THE APS, APPT AND ZONE 13 OF THE SPS
Houston TX.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 29-NOVEMBER 3, 2000

EASTERN ANALYTICAL SYMPOSIUM OF THE AMERICAN CHEMICAL SOCIETY
Atlantic City NJ.

Information: S. Gold, Eastern Analytical Symposium, P.O. Box 633, Montchanin, DE 19710 (302) 738-6218, Fax (302) 738-5275, http://www.eas.org

NOVEMBER 1-2, 2000

COMPUTATIONAL AND EXPERIMENTAL METHODS IN RECIPROCATING ENGINES
London UK.

Information: U. Otuonye, Conference and Events Department C587, Institution of Mechanical Engineers, 1 Birdcage Walk, London SW 1H 9JJ, UK, (0) 207-304-6864, Fax (0) 207-222-9881, e-mail: u_otuonye@imeche.org.uk

NOVEMBER 2-4, 2000

SOUTHEAST SECTION MEETING OF THE AMERICAN PHYSICAL SOCIETY
Starkville MS.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ NOVEMBER 3-4, 2000

9th CONFERENCE ON CURRENT TRENDS IN COMPUTATIONAL CHEMISTRY
Vicksburg MS.

Information: S.R. Allen, Jackson State University, Jackson, MS 39217, (601) 979-3723, e-mail: srallen@stallion.jsums.edu, http://www.ccl.net/cca/info/conferencelist/mess0665.shtml

♦ NOVEMBER 3-5, 2000

8th CONFERENCE ON MOLECULAR NANOTECHNOLOGY
Bethesda MD.

Information: Foresight Institute, Box 61058, Palo Alto, CA 94306, (650) 917-1122, Fax (650) 917-1123, http://www.foresight.org/conference

NOVEMBER 3-8, 2000

PHOTONICS EAST
Boston MA.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

NOVEMBER 5-10, 2000

ASME INTERNATIONAL MECHANICAL ENGINEERING CONFERENCE AND EXHIBITION
Orlando FL.

Symposia will Include:

- Symposium on Multiphase Flow in Biomedical Applications and Processes
- Dispersed Flows in Combustion, Incineration, and Propulsion Systems
- Application of Microfabrication to Fluid Mechanics

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 705-7037, Fax (212) 705-7143, http://www.asme.org

NOVEMBER 5-10, 2000

INTERNATIONAL SYMPOSIUM ON MULTIPHASE FLOW AND TRANSPORT PHENOMENA
Antalya, Turkey.

Topics will Include:

- Modeling of Multiphase Systems
- Transport Phenomena in Multiphase Systems
- Separation Phenomena, Processes and Equipment
- Measurement and Instrumentation
- Characteristic and Effective Properties of Multiphase Systems
- Bio-Aerosols and Bio-Systems
- Surface and Interfacial Phenomena
- Pollution Control Technology
- Clean Room Technology
- Multiphase Systems Applications
- Scaling Laws for Two-Phase Flow Phenomena
- Scaling Laws for Multiphase Flow

Information: D.M. Maron, Center for Technological Education Holon, POB 305, Holon 58102, Israel, (972) 3-502 6501, Fax (972) 3-502 6510, e-mail: barad_r@barley.cteh.ac.il, http://ichmt.me.metu.edu.tr/upcoming-meetings/MFTP-00/announce.html

NOVEMBER 5-10, 2000

UNITED ENGINEERING FOUNDATION CONFERENCE ON LEAN COMBUSTION TECHNOLOGY AND CONTROL
Santa Fe NM.

Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, e-mail: engfnd@aol.com http://www.engfnd.org/engfnd/conf.html, or from D. Dunn-Rankin, University of California at Irvine, CA, or R.K. Cheng, Lawrence Berkeley National Laboratory.

NOVEMBER 12-17, 2000

ANNUAL MEETING OF THE AMERICAN INSTITUTE OF CHEMICAL ENGINEERS
Los Angeles, CA.

Information: Meetings Department, American Institute of Chemical Engineers, United Engineering Center, 3 Park Avenue, New York, NY 10016, (212) 591-7325, Fax (212) 591-8894, e-mail: meetmail@aiche.org, http://www.aiche.org

NOVEMBER 13-18, 2000

EASTERN ANALYTICAL SYMPOSIUM OF THE AMERICAN CHEMICAL SOCIETY
Somerset NJ.

Information: S. Gold, Eastern Analytical Symposium, P.O. Box 633, Montchanin, DE 19710, (302) 738-6218, Fax (302) 738-5275, Web Site: http://www.eas.org

NOVEMBER 19-21, 2000

DIVISION OF FLUID DYNAMICS MEETING OF THE AMERICAN PHYSICAL SOCIETY
Washington DC.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

NOVEMBER 19-23, 2000

4th EUROMECH FLUID MECHANICS CONFERENCE
Eindhoven, The Netherlands.

Information: M.C.J. Tielemans, Fluid Dynamics Laboratory, Department of Physics, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands, e-mail: info@efmc2000.tue.nl, http://www.EFMC2000.TUE.NL

NOVEMBER 27-DECEMBER 1, 2000

FALL MEETING OF THE MATERIALS RESEARCH SOCIETY
Boston MA.

Information: Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (724) 779-3003, Fax (724) 779-8313, http://www.mrs.org

DECEMBER 3-9, 2000

6th RIO SYMPOSIUM ON ATOMIC SPECTROMETRY
Concepcion and Pucon, Chile.

Information: C.G. Bruhn, Departamento de Analisis Instrumental, Facultad de Farmacia, Universidad de Concepcion, P.O. Box 237, Concepcion, Chile, (56) 41-204252, Fax (56) 41-231903, e-mail: cbruhn@udec.cl, http://www.udec.cl/6riosymp/

DECEMBER 6-8, 2000

JOINT 52nd SOUTHEAST/56th SOUTHWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
New Orleans LA.

Information: A. Pepperman, SRRC, USDA-ARS, 1100 Robert E. Lee Boulevard, New Orleans, LA 70179, (208) 286-4510, Fax (208) 286-4367, e-mail: abpep@nola.srrc.usda.gov

DECEMBER 14-19, 2000

INTERNATIONAL CHEMICAL CONGRESS OF PACIFIC BASIN SOCIETIES
Honolulu HI.

Information: Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

♦ JANUARY 8-11, 2001

39th AIAA AEROSPACE SCIENCES MEETING AND EXHIBIT
Reno NV.

Information: S.X. Ying, MC 078-0421, The Boeing Company, 2401 E. Wardlow Rd., Long Beach, CA 90807, (562) 982-2113, Fax (562) 496-6647, e-mail: susan.x.ying@boeing.com, http://www.aiaa.org

♦ JANUARY 14-19, 2001

GORDON RESEARCH CONFERENCE ON MOLECULAR ENERGY TRANSFER
Harbortown Resort, Ventura CA.

Information: J. Bowman, Department of Chemistry, Emory University, 1515 Pierce Drive, Atlanta, GA 30322, e-mail: bowman@euch3g.chem.emory.edu, http://www.grc.uri.edu

♦ FEBRUARY 4-8, 2001

EUROPEAN WINTER CONFERENCE ON PLASMA SPECTROCHEMISTRY
Lillehammer, Norway.

Information: Y. Thomassen, NIOH, P.O. Box 8149 DEP, Oslo, Norway, N-0033, (47) 23-19 53 20, Fax (47) 23-19 52 06.

♦ FEBRUARY 18-23, 2001

GORDON RESEARCH CONFERENCE ON CHEMICAL REACTIONS AT SURFACES
Harbortown Resort, Ventura CA.

Information: J.C. Hemminger, Department of Chemistry, University of California, Irvine, CA 92697, e-mail: jchemmin@uci.edu, http://www.grc.uri.edu

♦ FEBRUARY 25 - MARCH 2, 2001

GORDON RESEARCH CONFERENCE ON GASEOUS IONS
Ventura Beach Hotel, Ventura CA.

Information: P. Armentrout, Chemistry Department, 315 S. 1400 E. Rm 2020, University of Utah, Salt Lake City, UT 84112, (801) 581-7885, Fax (801) 581-8433, e-mail: armentrout@chemistry.utah.edu, http://www.grc.uri.edu/programs/2001/gaseous htm

MARCH 4-8, 2001

THE PITTSBURGH CONFERENCE, PITTCON 2001
New Orleans LA.

Information: The Pittsburgh Conference, 300 Penn Center Boulevard, Suite 332, Pittsburgh, PA 15235, (412) 825-3220, Fax (412) 825-3224, e-mail: pittconinfo@pittcon.org, http://www.pittcon.org/

♦ MARCH 5-8, 2001

SOCIETY OF AUTOMOTIVE ENGINEERS WORLD CONGRESS
Detroit MI.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-1830, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

♦ MARCH 11-16, 2001

GORDON RESEARCH CONFERENCE ON MODERN DEVELOPMENTS IN THERMODYNAMICS
Ventura CA.

Information: R.S. Berry, Department of Chemistry, University of Chicago, 5735 South Ellis Avenue, Chicago, IL 60637, e-mail: berry@rainbow.uchicago.edu, http://www.grc.uri.edu

MARCH 12-16, 2001

ANNUAL MARCH MEETING OF THE AMERICAN PHYSICAL SOCIETY
Seattle WA.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MARCH 25-30, 2001

199th NATIONAL MEETING OF THE ELECTROCHEMICAL SOCIETY
Washington DC.

Information: The Electrochemical Society, Inc., Meetings Department, 10 South Main Street, Pennington, NJ 08534, (609) 737-1902, Fax (609) 737-2743, e-mail: ecs@electrochem.org, http://www.electrochem.org/meetings/199/meet.html

♦ MARCH 25-30, 2001

CONFERENCE ON STATIONARY SOURCE SAMPLING AND ANALYSIS FOR AIR POLLUTANTS XXV
Destin FL.

Information: B.K. Hickernell, United Engineering Foundation, Three Park Ave., 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, e-mail: engfnd@aol.com, http://www.engfnd/engfnd/1aw.html

APRIL 1-5, 2001

221st NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
San Diego CA.

Division of Fuel Chemistry:

- CO_2 Capture and/or Utilization Reaction Mechanisms in Fuel Processing
  P.F Britt, Chemistry Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831, (423) 574-5029, Fax (423) 576-5235, e-mail: brittpf@ornl.gov
- Coal Bed Methane
  P.C. Thakur, Consol Inc., R&D, 1027 Little Indian Creek Road, Morgantown, WV 26501, (304) 983-3207, Fax (304) 983-3209, e-mail: promodthakur@consolcoal.com
- Nitrogen Chemistry in Coal Utilization
  M.A. Wojtowicz, Advanced Fuel Research Inc., 87 Church Street, East Hartford, CT 06108, (860) 528-9806 ext 142, Fax (860) 528-0648, e-mail: marek@afrinc.com
- Hydrogen Energy
  R. Khan, Texaco Inc., P.O. Box 509, Beacon, NY 12508, (914) 838-7639, Fax (914) 838-7102
- Argonne National Lab Premium Coal Sample Database
  K. Vorres, 27 Windward Circle, Willowbrook, IL 60514, (630) 325-0931 [between Nov. 11 and April 15: 3432 North Applewood, Tucson, AZ 85712-5478, (520) 322-5256], e-mail: ksvorres@flash.net
- Carbon Products for Environmental Applications
  A. Lizzio, Illinois State Geological Survey, 615 East Peabody Drive, Champaign, IL 61801, (217) 244-4985, Fax (217) 333-8566, e-mail: lizzio@geoserv.isgs.uiuc.edu
- Fuels of the Future: Heavy Oil & Hydrogen for Fuel Cells
  R. Khan, Texaco Upstream Technology, 3901 Briar Park, Houston, TX 77042, (713) 954-6238, Fax (713) 954-6113, e-mail: khanmr@texaco.com
- Environmental Challenges for Fossil Fuel Combustion
  M.M. Maroto-Valer, Pennsylvania State University, Energy Institute, 405 Academic Activities Building, University Park, PA 16802, (814) 863-8265, Fax (814) 863-8892, e-mail: mmm23@psu.edu

APRIL 16-20, 2001

SPRING MEETING OF THE MATERIALS RESEARCH SOCIETY
San Francisco CA.

Information: Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (724) 779-3003, Fax (724) 779-8313, http://www.mrs.org

♦ APRIL 16-20, 2001

XIII CARIBBEAN CONFERENCE ON CHEMISTRY AND CHEMICAL ENGINEERING
Havana, Cuba.

Information: A.J. Nunez Selles, Sociedad Cubana de Quimica, Ave 21&200, Atabey, Apdo. 16042, Havana, Cuba, CP 11600, (537) 218-178, Fax (537) 336-471, cqf@infomed.sld.cu

APRIL 23-27, 2001

APRIL NATIONAL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Washington DC.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ APRIL 28 - MAY 1, 2001

2001 APRIL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Washington DC.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

APRIL 29-MAY 2, 2001

INTERNAL COMBUSTION ENGINE DIVISION SPRING TECHNICAL CONFERENCE OF THE AMERICAN SOCIETY OF MECHANICAL ENGINEERS
Philadelphia PA.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7054, Fax (212) 705-7143, http://www.asme.org

MAY 6-11, 2001

CLEO/QELS 2001
Baltimore MD.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, e-mail: confserv@osa.org, http://www.osa.org/mtg_conf

♦ MAY 7-9, 2001

CEC/SAE SPRING FUELS AND LUBRICANTS MEETING AND EXPOSITION
Orlando FL.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

♦ MAY 13-16, 2001

16th INTERNATIONAL CONFERENCE ON FLUIDIZED BED COMBUSTION
Reno NV.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 705-7037, Fax (212) 705-7143, http://www.asme.org

MAY 20-25, 2001

FLUIDIZATION X
Beijing, China.

Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, http://www.engfnd.org/engfnd/conf.html

MAY 20-25, 2001

2nd INTERNATIONAL SYMPOSIUM ON ADVANCES IN COMPUTATIONAL HEAT TRANSFER
Cairns, Australia.

Information: F. Arinc, Secretary-General, ICHMT, Mechanical Engineering Department, Middle East Technical University, 06531 Ankara, Turkey, (90) 312-210-1429, Fax (90) 312-210-1331, arinc@metu.edu.tr, http://ichmt.me.metu.edu.tr

♦ MAY 20-25, 2001

10th INTERNATIONAL CONFERENCE ON FLUIDIZATION: FLUIDIZATION FOR SUSTAINABLE DEVELOPMENT
Beijing, China.

Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, http://www.engfnd.org/engfnd/conf.html

MAY 27-JUNE 1, 2001

4th INTERNATIONAL CONFERENCE ON MULTIPHASE FLOW
New Orleans LA.

Information: E.E. Michaelides, School of Engineering, Tulane University, New Orleans, LA 70118, e-mail: icmf@mailhost.tcs.tulane.edu, http://mail.eng.lsu.edu/icmf.2001/
Deadline: Abstracts Due by July 1, 2000

MAY 30-JUNE 1, 2001

35th MIDDLE ATLANTIC REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Baltimore MD.

Information: L.J. Boucher, Towson University, Department of Chemistry, 8000 York Road, Towson, MD 21252-0001, (410) 830-3057, Fax (410) 830-4265, e-mail: lboucher@towson.edu

♦ JUNE 4-7, 2001

46th ASME INTERNATIONAL GAS TURBINE AND AEROENGINE TECHNICAL CONGRESS, EXPOSITION AND USERS SYMPOSIUM
New Orleans LA.

Information: A. Layne, National Energy Technology Center, DOE, 3610 Collins Ferry Road, MS CO2, Morgantown, WV 26505, (304) 285-4603, Fax (304) 285-4469, e-mail: abbie.layne@netl.doe.gov, http://www.asme.org

♦ JUNE 10-12, 2001

35th ASME NATIONAL HEAT TRANSFER CONFERENCE
Anaheim CA.

Information: C.B. Panchal, Energy Concept Co., Annapolis, MD 21401, (410) 266-6521, Fax (410) 266-6539, e-mail: cpanchal@aol.com, http://www.asme.org

JUNE 10-15, 2001

3rd INTERNATIONAL SYMPOSIUM ON RADIATIVE TRANSFER
Antalya, Turkey.

Information: F. Arinc, Secretary-General, ICHMT, Mechanical Engineering Department, Middle East Technical University, 06531 Anakara, Turkey, (90) 312-210-5214, Fax (90) 312-210-1331, http://ichmt.me.metu.edu.tr
Deadline: 4 Copies of Manuscript Due by December 15, 2000.

JUNE 11-13, 2001

JOINT CENTRAL/GREAT LAKES REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Grand Rapids MI.

Information: R.J. McCabe, Parke-Davis Pharmaceuticals, 188 Howard Ave., Holland, MI 49424, (616) 392-2375 ext. 2386, Fax (616) 392-8916, e-mail: Richard.McCabe@wl.com

♦ JUNE 11-14, 2001

19th AIAA APPLIED AERODYNAMICS CONFERENCE
15th AIAA COMPUTATIONAL FLUID DYNAMICS CONFERENCE
31st AIAA FLUID DYNAMICS CONFERENCE
32nd AIAA PLASMADYNAMICS AND LASERS CONFERENCE
35th AIAA THERMOPHYSICS CONFERENCE
Anaheim CA.

Information: Meetings Department, American Institute of Aeronautics and Astronautics, 1801 Alexander Bell Drive, Suite 500, Reston, VA 20191, (703) 264-7500 or (800) 639-2422, e-mail: custserv@aiaa.org, http://www.aiaa.org

JUNE 13-15, 2001

JOINT 33rd CENTRAL/33rd GREAT LAKES REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Grand Rapids MI.

Information: R.J. McCabe, Parke-Davis, 188 Howard Avenue, Holland, MI 49423, (616) 392-2375 ext 2386, Fax (616) 392-8916, e-mail: Richard.McCabe@wl.com

JUNE 13-16, 2001

56th NORTHWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Seattle WA.

Information: S. Jackels, Department of Chemistry, Seattle University, 900 Broadway, Seattle, WA 98122, (206) 296-5946, Fax (206) 296-5786, e-mail: sjackels@seattleu.edu

♦ JUNE 17-22, 2001

GORDON RESEARCH CONFERENCE ON ATMOSPHERIC CHEMISTRY
Salve Regina University, Newport RI.

Information: S.P. Sander, Jet Propulsion Laboratory, Mail Stop 183-901, 4800 Oak Grove Drive, Pasadena, CA 91109, e-mail: stanley.sander@jpl.nasa.gov, http://www.grc.uri.edu

♦ JUNE 23-28, 2001

GORDON RESEARCH CONFERENCE ON ANALYTICAL CHEMISTRY
Connecticut College, New London CT.

Information: P.W. Bohn, Department of Chemistry, University of Illinois, 600 South Mathews, Urbana, IL 61801, e-mail: bohn@aries.scs.uiuc.edu, http://www.grc.uri.edu

JUNE 24-27, 2001

30th NORTHEAST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Durham NH.

Information: H. Mayne, Chemistry Department, University of New Hampshire, (603) 862-1550, e-mail: howard.mayne@unh.edu

JUNE 24-28, 2001

ANNUAL MEETING OF THE AIR AND WASTE MANAGEMENT ASSOCIATION
Orlando FL.

Information: Air and Waste Management Association, Member Services, One Gateway Center, Third Floor, Pittsburgh, PA 15222, (800) 270-3444 or (412) 232-3444, Fax (412) 232-3450, http://www.awma.org

JULY 1-6, 2001

GORDON RESEARCH CONFERENCE ON LASER DIAGNOSTICS IN COMBUSTION
Mount Holyoke College, South Hadley MA.

Information: J.B. Jeffries, Molecular Physics Laboratory, SRI International, 333 Ravenswood Ave., Menlo Park, CA 94025, (650) 859-6341, Fax (650) 859-6196, e-mail: jay.jeffries@sri.com

♦ JULY 8-11, 2001

37th AIAA/ASME/SAE/ASEE JOINT PROPULSION CONFERENCE
Salt Lake City UT.

Information: Meetings Department, American Institute of Aeronautics and Astronautics, 1801 Alexander Bell Drive, Suite 500, Reston, VA 20191, (703) 264-7500 or (800) 639-2422, e-mail: custserv@aiaa.org, http://www.aiaa.org

♦ JULY 8-13, 2001

GORDON RESEARCH CONFERENCE ON GRAVITATIONAL EFFECTS IN PHYSICO-CHEMICAL SYSTEMS
Colby-Sawyer College, New London NH.

Information: P.H. Steen, Department of Chemical Engineering, Cornell University, 346 Olin Hall, Ithaca, NY 14853, e-mail: phs7@cornell.edu, http://www.grc.uri.edu

♦ JULY 8-13, 2001

GORDON RESEARCH CONFERENCE ON PHOTOIONS, PHOTOIONIZATION AND PHOTODETACHMENT
Williams College, Williamstown MA.

Information: M. Johnson, Department of Chemistry, Yale University, P.O. Box 208107, New Haven, CT 06520, e-mail: Mark.johnson@yale.edu, http://www.grc.uri.edu

JULY 9-11, 2001

COMBUSTION CHEMISTRY: ELEMENTARY REACTIONS TO MACROSCOPIC PROCESSES: FARADAY DISCUSSION NUMBER 119
Leeds, UK.

Joint Meeting with the British Section of the Combustion Institute.
Information: M. Pilling, School of Chemistry, University of Leeds, Leeds UK, e-mail: m.j.pilling@chem.leeds.ac.uk, http://www.chem.leeds.ac.uk

♦ JULY 22-27, 2001

GORDON RESEARCH CONFERENCE ON HIGH TEMPERATURE CORROSION
Colby-Sawyer College, New London NH.

Information: P.Y. Hou, Lawrence Berkeley National Laboratory, Materials Science Division, 1 Cyclotron Road, MS 62-203, Berkeley, CA 94720, e-mail: pyhou@lbl.gov, http://www.grc.uri.edu

JULY 29-AUGUST 2, 2001

36th INTERSOCIETY ENERGY CONVERSION ENGINEERING CONFERENCE
Savannah GA.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7057, Fax (212) 705-7143, http://www.asme.org

♦ AUGUST 6-10, 2001

INTERNATIONAL CONGRESS ON ANALYTICAL SCIENCES 2001
Yokohama, Japan.

Information: T. Sawada, Chairman, Department of Applied Chemistry, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo, Japan 113-8656, (81) 3-5841-7236, ext. 7237, Fax (81) 3-5841-6037, e-mail: icas2001@laser.t.u-tokyo.ac.jp, http://wwwsoc.nacsis.ac.jp/jsac/icas2001/

AUGUST 19-24, 2001

1st INTERNATIONAL CONFERENCE ON ADVANCED VIBRATIONAL SPECTROSCOPY
Turku, Finland.

Information: M. Hotokka, Department of Physical Chemistry, Abo Akademi University, FIN-20500 Turku, Finland, 358-2-215-4295, Fax 358-2-215-4706, e-mail: icavs@abo.fi, http://www.abo.fi/icavs

♦ AUGUST 19-24, 2001

GORDON RESEARCH CONFERENCE ON PHOTOACOUSTIC AND PHOTOTHERMAL PHENOMENA
Queen's College, Oxford UK.

Information: D. Fournier, UPMC/CNRS, Laboratoire d'Instrumentation, 10 Rue Vaugelin, Paris 75005, France, e-mail: fournier@optique.espci.fr, http://www.grc.uri.edu

AUGUST 20-24, 2001

13th INTERNATIONAL CONFERENCE ON FOURIER TRANSFORM SPECTROSCOPY
Turku, Finland.

Information: M. Hotokka, Department of Physical Chemistry, Abo Akademi University, FIN-20500 Turku, Finland, (358) 2-265-4295, Fax (358) 2-265-4706, e-mail: icofts@abo.fi, http://www.abo.fi/icofts

AUGUST 26-30, 2001

222nd NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Chicago IL.

Division of Fuel Science:

- Cofiring or Coprocessing Coal & Biomass
  J.T. Cobb, Jr., University of Pittsburgh, Chemical Engineering Department, 1137 Benedum Hall, Pittsburgh, PA 15261, (412) 624-7443, Fax (412) 624-9639, e-mail: cobb@engrng.pitt.edu
- Computer Modeling in Fuel Chemistry
  J. Mathews, Pennsylvania State University, Energy & Geo-Environmental Engineering Department, 151 Hosler Building, University Park, PA 16802, (814) 863-6213, Fax (814) 865-3248, e-mail: jpm10@psu.edu; M.T. Klein, Rutgers, State University of New Jersey, School of Engineering, Office of the Dean, B204, 98 Bret Road, Piscataway, NJ 08854-8058, (732) 445-4453, Fax (732) 445-7067, e-mail: mtklein@jove.rutgers.edu
- Fine Particulate (PM2.5) Formation & Emissons from Fuel Combustion
  C.M. White, Department of Energy, Federal Energy Technology Center, Mail Stop 94-212, P.O. Box 10940, Pittsburgh, PA 15236, (412) 386-5808, Fax (412) 386-4158, e-mail: cwhite@fetc.doe.gov
- Catalysis in Fuel Processing for Fuel Cell Application
  S.P. Katikaneni, Fuel Cell Energy, Advanced Technology Group, 3 Great Pasture Road, Danbury, CT 06813, (203) 825-6067, Fax (203) 825-6150, e-mail: skatikaneni@fce.com; A.M. Gaffney, DuPont Central R&D, Experimental Station, P.O. Box 80262, Wilmington, DE 19880, (302) 695-1800, Fax (302) 695-8347, e-mail: anne.m.gaffney@usa.dupont.com; C. Song, Pennsylvania State University, Energy & Geo-Environmental Engineering, 206 Hosler Building University Park, PA 16802, (814) 863-4466, Fax (814) 865-3248, e-mail: csong@psu.edu
- Value-Added Carbon Products from Fossil Fuels
  F. Rusinko, Pennsylvania State University, Energy Institute 407 Academic Activities Building, University Park, PA 16802, (814) 863-8085, Fax (814) 865-8892, e-mail: fjr4@psu.edu; J.W. Zondlo, College of Engineering & Mineral Resources, Department of Chemical Engineering, P.O. Box 6102, Morgantown, WV 26506; B. Tomer, Department of Energy, Federal Energy Technology Center, 3610 Collins Ferry Road, P.O. Box 88, Morgantown, WV 26507.
- Mercury Emissions from Coal
  K. Katrinak, Microbeam Technologies, 1521-24th Avenue S., Suite B-2, Grand Forks, ND 58201, (701) 772-4482, Fax (701) 772-4099, e-mail: katrinak@badlands.nodak.edu; K. Galbreath, University of North Dakota, Energy & Environmental Research Center, P.O. Box 9018, Grand Forks, ND 58202, (701) 777-5127, Fax (701) 777-5181, e-mail: kgalbreath@eerc.und.nodak.edu
- General Fuel Chemistry
  S.V. Pisupati, Pennsylvania State University, Energy & Geo-Environmental Engineering, 124 Hosler Building, University Park, PA 16802, (814) 865-0874, Fax (814) 865-3248, e-mail: sxp17@psu.edu

Information: Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org
Deadline: Electronic Abstract Submissions (preferred) or 4 Hard Copies of 150-word Abstract (original on ACS Abstract Form) Due to Symposium Organizers by April 15, 2001. Preprints Due to Symposium Chairs by May 15, 2001.

SEPTEMBER 2-7, 2001

200th NATIONAL MEETING OF THE ELECTROCHEMICAL SOCIETY AND THE 52nd MEETING OF THE INTERNATIONAL SOCIETY OF ELECTROCHEMISTRY
San Francisco CA.

Information: The Electrochemical Society, Inc., Meetings Department, 10 South Main Street, Pennington, NJ 08534, (609) 737-1902, Fax (609) 737-2743, e-mail: ecs@electrochem.org, http://www.electrochem.org/meetings/198/meet.html

SEPTEMBER 23-27, 2001

52nd SOUTHEAST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Savannah GA.

Information: G. Novotnak, Kemira Pigments, 104 Carlton Road, Savannah, GA 31410, (912) 652-1290, Fax (912) 897-1163, e-mail: george.novotnak@kemira.com

SEPTEMBER 23-27, 2001

6th WORLD CONGRESS OF CHEMICAL ENGINEERING: A NEW CENTURY OF CHEMICAL ENGINEERING
Melbourne, Australia.

Information: Meetings Department, American Institute of Chemical Engineers, United Engineering Center, 3 Park Avenue, New York, NY 10016, (212) 591-7325 or (800) 242-4363, Fax (212) 591-8894, e-mail: meetmail@aiche.org, http://www.aiche.org

SEPTEMBER 24-26, 2001

INTERNAL COMBUSTION ENGINE DIVISION FALL TECHNICAL MEETING OF THE AMERICAN SOCIETY OF MECHANICAL ENGINEERS
Argonne IL.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7054, Fax (212) 705-7143, http://www.asme.org

♦ SEPTEMBER 24-27, 2001

INTERNATIONAL SAE FALL FUELS AND LUBRICANTS MEETING AND EXPOSITION
San Antonio TX.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

SEPTEMBER 24-28, 2001

5th WORLD CONFERENCE ON EXPERIMENTAL HEAT TRANSFER, FLUID MECHANICS AND THERMODYNAMICS
Thessaloniki, Greece.

Information: G.P. Celata, Conference Chairman, ENEA Casaccia, Via Anguillarese 301, I-00060 S.M. Galeria, Rome, Italy, (39) 06-30483905, Fax (39) 06-30483026, e-mail: celata@casaccia.enea.it, http://www.ing.unipi.it/exhft5
Deadline: Abstract Due by July 28, 2000

OCTOBER 5-12, 2001

28th ANNUAL MEETING OF THE FEDERATION OF ANALYTICAL CHEMISTRY AND SPECTROSCOPY SOCIETIES
Detroit MI.

Information: C. Lilly, Federation of Analytical Chemistry and Spectroscopy Societies, 1201 Don Diego Ave., Santa Fe, NM 87505, (505) 820-1648, Fax (505) 989-1073, e-mail: jsjoberg@trail.com, http://facss.org/info.html

OCTOBER 10-13, 2001

36th MIDWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Lincoln NE.

Information: D. Berkowitz, Department of Chemistry, University of Nebraska, Lincoln, NE 68588-0304, (402) 472-2738, Fax (402) 472-9402, e-mail: dbb@unlinfo.edu

♦ OCTOBER 14-18, 2001

6th INTERNATIONAL SYMPOSIUM ON SELF PROPAGATING HIGH TEMPERATURE SYNTHESIS
Haifa, Israel.

Information: I. Gotman, Technion-Israel Institute of Technology, Department of Materials Engineering, Technion, Haifa, Israel 32000, (972) 4-829-2112, Fax (972) 4-832-1978, e-mail: gotman@techunix.technion.ac.il, http://www.technion.ac.il/technion/materials/conferences.html

OCTOBER 14-19, 2001

INTERNATIONAL SYMPOSIUM ON VISUALIZATION AND IMAGING IN TRANSPORT
Antalya, Turkey.

Information: F. Arinc, Secretary-General, ICHMT, Mechanical Engineering Department, Middle East Technical University, 06531 Ankara, Turkey, (90) 312-210-1429, Fax (90) 312-210-1331, arinc@metu.edu.tr, http://ichmt.me.metu.edu.tr

OCTOBER 16-19, 2001

57th SOUTHWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
San Antonio TX.

Information: S.T. Weintraub, Department of Biochemistry, University of Texas Health Science Center, 7703 Floyd Curl Drive, San Antonio, TX 78284, (210) 567-4043, Fax (210) 567-5524, e-mail: weintraub@uthscsa.edu

OCTOBER 23-26, 2001

36th WESTERN REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Ventura CA.

Information: R.W. Hurst, 9 Faculty Court, Thousand Oaks, CA 91360, (805) 492-7764, Fax (805) 241-7149, e-mail: Alarwh@aol.com

NOVEMBER 26-30, 2001

FALL MEETING OF THE MATERIALS RESEARCH SOCIETY
Boston MA.

Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (724) 779-3003, Fax (724) 779-8313, e-mail: info@mrs.org

♦ NOVEMBER 28-30, 2001

2001 SAE SMALL ENGINE TECHNOLOGY CONFERENCE AND EXPOSITION
Pisa, Italy.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org
Submit your abstract of up to 500 words by November 2, 2000 to Karin Bolcshazy, SAE International, 400 Commonwealth Drive, Warrendale, PA 15096, (724) 772-7179, Fax (724) 776-1830, e-mail: karinb@sae.org
The abstract should include a tentative paper title, authors and co-authors (full names, position, company address, email, telephone and fax numbers).

MARCH 18-22, 2002

MARCH MEETING OF THE AMERICAN PHYSICAL SOCIETY
Indianapolis IN.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ MARCH 18-22, 2002

PITTCON 2000: THE PITTSBURGH CONFERENCE
New Orleans LA.

Information: The Pittsburgh Conference, 300 Penn Center Blvd., Suite 332, Pittsburgh, PA 15235, (412) 825-3220, Fax (412) 825-3224, e-mail: pittconinfo@pittcon.org, http://www.pitcon.org/

♦ APRIL 7-12, 2002

223rd NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Orlando FL.

Information: Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

CURRENT BIBLIOGRAPHY RELEVANT TO FUNDAMENTAL COMBUSTION

February 2000

Keith Schofield, ChemData Research, P.O. Box 40481
Santa Barbara, CA 93140, (805) 966-7768, Fax (805) 893-8797
e-mail: combust@mrl.ucsb.edu
http://www.ca.sandia.gov/CRF/Publications/CRB/CRB.html

1. FUELS/SYNFUELS - GENERAL

84203. Touryan, K.J., "Renewable Energy: Rapidly Maturing Technology for the 21st Century," *J. Propulsion Power* 15, 163-174 (1999).
Renewable Energy Sources Trends Technology Feasibility

84204. Gupta, A.K., and D.G. Lilley, "Energy Recovery Opportunities from Wastes," *J. Propulsion Power* 15, 175-180 (1999).
Waste Fuels Energy Recovery Technologies

84205. Miller, C.A., and R.K. Srivastava, "The Combustion of Orimulsion and Its Generation of Air Pollutants," *Prog. Energy Combust. Sci.* 26, 131-160 (2000).
Bitumen/Oil Emulsified Fuel Combustion Emissions

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Upgraded Biomass Derived Fuels Methods Yields

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Biomass Fuels Sawdust Combustion Ash Analysis High Na,K Emissions

(84460) Diesel Engine Performance, Emissions — Biofuel/Diesel Fuels

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2. LIQUEFACTION/GASIFICATION

84213. Yoshikawa, K., H. Katsushima, M. Kasahara, T. Hasagawa, R. Tanaka and T. Ootsuka, "Innovative Coal Gasification System with High Temperature Air," pp. 932-937 in *IECEC-97: Proceedings of the 32nd Intersociety Energy Conversion Engineering Conference. Volume 2*, pp. 768-1542, 135 Papers Presented in Honolulu HI, August 1997, American Institute of Chemical Engineers, New York NY (1997). — Gasification; Coal; High Temperature Air Method

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Gasification
Biomass
Fuel 'N' Release
Kinetic Model
Simulation

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Gasification
Biomass
Fuel 'N' Release

3. BURNERS

(See also Section 21 for Burner Emissions and Incinerator Performance)

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Utility Boiler
Convective Section
Heat Transfer
Model

84220. Coelho, P.J., "Mathematical Modeling of the Convection Chamber of a Utility Boiler: The Theory," *Numer. Heat Transfer A. Applications* 36, 429-447 (1999).

Utility Boiler
Convection Chamber
Heat Transfer
Modeling

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Porous Matrix
Combustor
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Modeling

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Ceramic Honeycomb
Preheated Air
Furnace
Low NO_x Emissions

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Catalytic
Radiant Burner
CH_3OH/H_2
Fuel
Emissions

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Catalytic
Combustor
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Stability
NO_x Emissions

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Catalytic
Domestic
CH_4 Burner
NO_x Emissions

(84381) Turbulence Generating Flows, LDV

Cruciform Burner

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New Burner Concept
Ni Metal
Combustor
Ni/O_2 Oxidation
NiO/CH_4 Reduction
Separate Cycles
Low Emissions

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Combustors
Natural Gas
Cyclone/Swirl
Wide Range Burners
Low NO_x
LDA Flowfields

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Rich/Quick Mix/
Lean Combustor
Crossflow Air
Injection
Low NO_x

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Effects

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Sulfur Release
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Effects

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Turbulent Flame
Propagation
Speeds

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Co-firing
Options

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Combustion
Performance
NO_x ,SO_2 Emissions

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Vaporization
Ignition
Transient
Modeling

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Vaporization
Mixing
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Vaporization
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Combustion
Heat Transfer
Interactions
Modeling

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Evaporation
Surface
Temperature
C_6-C_{10} Alkanes
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Ignition
C_7H_{16}
Modeling

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Ignition
Hot Stagnant Air
Numerical
Modeling

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n-C_7H_{16}/Air

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Extinction
Heat Transfer
Modeling

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Rich CH_3OH
Stretched
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Modeling

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Flame Spread
OH* Emission
Gravity,Pressure
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Multicomponent
Surface Regression
Thin Flame
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Combustion
P,T Effects

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Combustion
Blended Fuel
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OH* Imaging

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C_7H_{16}/Air
Saturated LIF
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n-RH/*n*-$C_{16}H_{34}$
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Biomass Oils
CH_3OH,H_2O Additive Effects
Microexplosions

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Droplet Combustion
Cenosphere Formation

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Metal Combustion
Phase Changes
Al,Cu,Fe
Mg,Zr
Disruptions

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Al Droplet Combustion
Normal
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Al,Ti/O_2
Ti/N_2
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Chemical Equilibrium
Controlling Aspects

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TNAZ
Pyrolysis
Products
Kinetic Control
IR Frequencies
Thermodynamic Properties
0-1500 K

(84415) Fire Retardants, Char Formation, Yields, Review

Polymers

(84535) Soot Formation, Yields

Plastic Polymer
Combustion

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Pyrolysis
Fluidized Bed
Products

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PMMA
Diffusion Flame
Characterization

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(84458) Temperatures, Diesel Engines, In-Cylinder, CCD Imaging — 2-Color Pyrometer

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NO Formation

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Natural Gas
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Modulation
Method

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Instabilities

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Operating
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Natural Gas
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OH* Monitor
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Gas Turbines
Lean Mode
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Diffusion Flame
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Modeling

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Diffusion Flames
CO_2, N_2 Additives
Control

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H_2/Air
Diffusion Flames
Acoustic
Instabilities
NO Formation
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Mechanisms

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Self-ignition
Stability

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Limits
$H_2/O_2/CO_2$
Opposed Jet
Stretch Effects
Modeling

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$CO/H_2/N_2$
Rayleigh,Raman
T,OH,NO LIF
LDV
Scalar Structure

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Emissions
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CH_4 /Air
Structure

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Countergradient
Diffusion
Velocity Spectrum

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CH_4/Air
CO,NO_x
Emissions
Added Fuel
Effects

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Interactions
Oil Smoke
Visualization
Mixing

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Tube Flame
Overpressure
Generation

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Pressure
Suppression

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Explosive
Dissociation
AgN_3, TlN_3
PbN_6
Luminescence
Spectra

14. FLOW PHENOMENA/VELOCITIES/DIFFUSION

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Maximum
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PIV
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Swirl Spray
Nozzle Flowfield
3-D Velocities
Wind Tunnel
Car Wakes

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Swirling Combustor
Fuel/Air
Mixing
LDA Measurements

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LDA

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Supersonic
H_2/Air
Mixing Layers
Model

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(84354)	H_2 Jet, Supersonic Heated Crossflow Air, Stabilities, OH PLIF	Schlieren Flowfield
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Rate Constants
T Dependence
Review

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$Ar(^3P) + CH_3Cl$
Orientation
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$CClF_3.N_2 + e^-$
$CHF_3.N_2 + e^-$
Attachment
Rate Constants

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$CO^+ + CH_4$
$N_2O^+ + CH_4$

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$Cl^+ + C_2H_2$
Barrier Free
Channels
Calculations

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$C_2HCl_3 + e^-$
Air Mixture
Destruction
Efficiencies
Products

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Soot Formation

(84972) Vibrational Relaxation, Rate Constants

$HCN^+(v) + He$
$DCN^+(v) + He$

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Rotational
Alignment
Drift Tube
Calculations

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$NO^+, O_2^+ + M$
$O^+, N^+, N_2^+ + M$
Rate Constants
Branching Ratios
M=4 Alkylbenzenes

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$N_2(v) + e^-$

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$Na_3^+ + He$
Fragmentation
Channels
Cross Sections

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$O^+ + NO$
Cross Sections
3 Channels
Reactant Energy
Thresholds

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$PH_2^+ + PH_3$
$PH_3^+ + PH_3$
Rate Constants
Product Ions
Measurements
$\Delta H_f(P_2H_n^+)$
n=1-6,Calculations

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$S^+ + M$
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M=20 Organics
Ion Products

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$SiNCO^+$
$SiNCS^+$
Ionized Neutrals
Mass Spectrometry
Stabilities

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Fire Suppression
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State of the Art
Review

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Fire Retardants
Polymers
Char Formation
Yields
Review

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Amino-Additives

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(84465)	NO_x Control, Diesel Engine Exhaust, Discharge/Catalyst Treatment	CH_3ONO_2 Additive
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(84702)	Effects, $(CH_3)_2O/O_2$ Flow Reactor, Kinetic Modeling	NO,NO_2 Additives

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Heterogeneous
$ClONO_2/HCl(H_2O)_n$
Reactivities
Cluster
Enhancements

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Heterogeneous
$HCl,HBr/H_2O(l)$
$HI/H_2O(l)$
Uptake
Coefficients

(84593) FTIR Spectra, Mixtures

HNO_3, H_2SO_4
Aqueous Films

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Heterogeneous
$NO_3/NaBr(s)$
$NO_3/NaCl(s)$
Uptake
Coefficients
T Dependences

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I.C. Engines
High Pressure
Direct Injection
Performance
Improvements
Review

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I.C. Engine
Droplet Sizing
Scattering Method

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I.C. Engine
Natural Gas
Lean Burn
Ignition Delay
Characterization

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I.C. Engine
Port Injected
Fuel/Vapor
Distributions
Exciplex PLIF

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I.C. Engine
DI Gasoline
2-D Mapping
LIF,$(CH_3)_2CO$
Tracer

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I.C. Engine
Cycle-to-Cycle
Idling Variations
Controlling Factors

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I.C. Engine
Fuel Lean
Instabilities
Behavioral
Patterns

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I.C. Engine
CH_4 Fueled
H_2 Additive
Effects

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I.C. Engine
Velocities
Spark Plug Region
2-Color PIV
Turbulence

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I.C. Engine
2-Stroke
OH* Emission
EGR Effects
Auto-ignition

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I.C. Engines
Unburnt
Hydrocarbon Emissions
IR Absorption
Monitoring Method
FID Comparisons

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I.C. Engine
Crevice UHC
Emissions
PLIF
Dependences

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I.C. Engine
Unburned Hydrocarbons
Inter-ring Crevice Effects

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C_5H_8 Emissions

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I.C. Engine
Natural Gas
Direct Injection
NO_x Emissions

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I.C. Engines
CO,HC,NO_x Emissions
Predictive
Generic Functions

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I.C. Engines
NO Formation
Stratified EGR/Air Effects

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I.C. Engine
NO,LIF
Profiles
Measurements
Modeling

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I.C. Engine
NO,PLIF
Equivalence Ratio Effects
In-Cylinder Measurements

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I.C. Engine
PIV Flowfields
PLIF,NO Measurements
Modeling

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N_2O Emissions

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I.C. Engines
Soot Formation
Liquid Fuel
Equivalence Ratio Effects

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I.C. Engines
Soot Formation
Fuel,Oil
Catalytic Converter
Dependences

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I.C. Engines
Soot Formation
Mechanisms
Model

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Vehicular
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Fuels/Emissions
Comparisons

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Engine Emissions
Fine Particles
Extinction/
Scattering
Measurements

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MMT Fuel Additive
Mn Particle
Emissions
Sizes
Composition

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Diesel Engines
Auto-ignition
Direct Injection
Spray Model

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Diesel Engine
Indirect Injection
Engine Noise
EGR Effects

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Natural Gas/Air
Injection
Performance

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Diesel Engine
$(CH_3)_2O$
Direct Injection
Performance

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Diesel Engine
Coconut Oils
Testing

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Diesel Engines
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2-Color Pyrometry
In-cylinder
CCD Imaging

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Diesel Engines
Synfuel
Emissions
Performance

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Diesel Engine
Biofuel/Diesel
Performance
Emissions

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Diesel Engine
NO Emissions
Model

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Diesel Engine
NO_x ,Hydrocarbon
Emissions
H_2O_2 ,H_2O
Injection Effects

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Diesel Engine
Multistaged
NO_x Emission
Reductions

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NO_x Control
Catalytic
Converter
Lean Burn
Modeling

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Diesel Engine
NO_x Control
CH_3ONO_2 Addition
Discharge/
Catalyst

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Diesel Engines
Exhaust
Dilution
Particle
Size Distribution
Effects

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Particle Emissions
Laser Mass Analysis
Potential
Measurement
Artifacts

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Diesel Engines
Soot Traps
Regeneration
Modes

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$(CH_3)_2S$,OCS
CS_2 ,H_2S
Sources/Sinks
Budgets

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Atmospheric
C_5H_8
Anthropogenic
Contributions
Vehicle Role

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$C_3H_7OC_2H_4OH$

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PAHS
Vehicular
Contributions

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Incineration
CH_2Cl_2
Postflame Region
Injection
Products
Kinetics

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CO_2 Control
Flue Gas
Separation
CaO Absorber

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Destruction
t-$C_4H_9OCH_3/H_2O$
Contaminated
Water
Ultrasonics/O_3
Method

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Tar Volatiles
Combustion
Flow Reactor
FTIR Analysis
N-Species
Formation

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Incineration
Solid Wastes
Organic Emissions
Formation

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PAH
Growth
Reaction Dynamic
Pathways
Modeling

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PAH
Formation
CH_4/Air
Mass Analysis
Sequences

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C_6H_6,PAH
Formation

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PAH Emissions
Diesel Fuel
Open Burn

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PAH,Organics
Formation
$C_{10}H_8/O_2/Ar$
Near Sooting Flame
Sampling
Analysis

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Incineration
Medical Waste
Emissions
PAHS

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Combustion
Fuel Stoves
PAH,Particle
Emissions

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Furans
Formation
C_6H_5OH/O_2
$C_6H_4(Cl)OH/O_2$
Flow Reactor
Mechanisms

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Dioxin
Formation
C_2H_2/HCl/CuO
Catalyzed
Pathways

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Incineration
PCDD,PCDF
Aromatics
Secondary
Flue Gas
Formation

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Incineration
Heavy Metal
Emissions
Sorbents
Cl Additive
Effects

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Heavy Metal
Combustion
Emissions
Aerosols
Coagulation
Cd,Ni,Pb

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NO_x Control
Thermal NH_3 Process
Kinetic Modeling
NH_2+NO
Branching Inclusion
Adequacies

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NO Control
Natural Gas
Reburn Method
Mixing Effects

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Staged Combustion
Kinetic Modeling
Reburn Location

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NO_x Control
Gas Reburn
Coal Boilers
Automatic
Controller

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NO Control
NH_3/Cu
Zeolite
Method
Efficiencies

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NO Control
Catalytic
Methods
$(NO)_3$,$(NO)_3^-$
Roles

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NO_x Control
Flue Gases
Discharge Method
Multipoint
Electrode

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NO_x ,SO_2 Control
Flue Gases
Discharge Method
C_3H_6 ,NH_3 Additive
Effects

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Emissions Control
Pulsed Discharge
Method
CO_2 ,NO_x ,SO_2
Particulates

(84212) Gaseous Fuels, Technologies, Review — Desulfurization

22. SOOT, DIAMOND, PARTICLE FORMATION/CONTROL

(See also Section 19 for Soot Formation in Engines and Section 21 for Combustion Generated Soot and Particle Formation)

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23. PARTICLE CHARACTERIZATION

(See also Section 5 for Spray Characterization)

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(84466) Diesel Engine Exhaust Dilution Effects — Particle Sizes

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(84452)	Composition, I.C. Engine, Methylcyclopentadienyl Manganese Tricarbonyl Octane Improver	Mn Particle Sizes
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(84209)	Sawdust, Sander-dust Combustion, Na, K Emissions	Ash Analysis
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(See also Section 22 for Nucleation and Growth of Particles)

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(84503)	Heavy Metal Combustion Emissions, Cd, Ni, Pb	Aerosol Coagulation

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Fullerene
Nanotube
Formation
Coal Source
Analysis

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C_n
Nanotubes
Formation
$Fe(CO)_5/CO$
Pyrolysis

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C_n,PAH
Flame Formation
C_6H_6/O_2
Profiles
Pathways
PAH/Soot
Correlations

(84951) Structural Calculations, Electronic Description

C_{20}

(84952) Structural Calculations, Frequency Assignments, Data Comparisons

C_{60} ,C_{60}^{6-}

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C_{60}
fs Photoionization
Fragmentation
Mass Analysis

(85010) Absorption Spectrum, Calculations

IP,EA(C_{60})

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C_{60} ,C_{70}
$C_{60}O$,$C_{70}O$
Flame Formation
C_6H_6/O_2
Sampling/Analysis

(84964) Structural Calculations, Geometry, D_0

$(NH_3)_2$

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Cluster Growth
V_2O,V_2O_2
Ti_2O_2 ,Ti_2O_3
Dynamics
TOF Monitor

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Flame Radiation
Turbulent
Fluctuation
Effects

(84422) Nongray, Soot Influence, Heat Transfer Modeling — Furnace Radiation

(84816) Chemiluminescence, $Ca(^1D_2) + HCl,HBr$, Product Cross Section Dependences — CaCl(A) CaBr(B,A)

(84618) Chemiluminescence, Photon Yields, $Ca(^1D,^3P) + CX_{4-n}Y_n$, X,Y=F,Cl,Br — CaX(B,A-X)

(84863) Dioxirane (Cyclic Peroxide) Formation, Chemiluminescence, Review — $RR'O_2$

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CCl_3NO_2
Rotational Spectrum
Constants
Dipole Moment

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$CD_2Se(a\text{-}X)$
Laser Induced
Phosphorescence
Spectral Constants

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CF_2I_2
CH_2I_2
Low-lying
Electronic States
UV Transitions
Calculations

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HCO
Rydberg States
Double Resonance
Absorption
Spectrum
Vibrational
Autoionization
Linewidths

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CH_3F,CH_3Cl
CH_3Br,CH_3I
FTIR Spectra
Overtones
Frequencies
Assignments

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CH_nOH_m,$CH_nOH_m^+$
IR Spectra
Frequencies
Calculations

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$CH_3O(X)$,$RO(A,X)$
$R=C_2H_5$,C_3H_7,C_4H_9
Vibronic Structure
EA,$\Delta H_f(RO)$
$D(ROH)$,$\Delta H_f(RO^{\pm})$
Anion PES

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$CO(v\leq 6,J)$
Cooled Discharge
FTIR Spectra
High Rotational
Excitation

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CO
IR Spectra
$v \leq 12, \Delta v = 1$
Overlapping Bands
Pattern Recognition Algorithm

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CS^+(A-X)
Absorption
Velocity Modulation
Constants

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$(CHO)_2$,$(T_1\text{-}S_0)$
Phosphorescence
Spectra
Constants
Jet Cooled

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C_2H_3(A-X)
Absorption
Cross Sections
Cavity Ringdown

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$C_2H_5(\nu_{CH2})$
IR Laser
Absorption
Spectrum
Jet Cooled
Assignments

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C_2H_5SCl
Photoionization
Spectrum
IP
Vibrational
Frequencies

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C_2H_6
IR,Raman
4500-6500 cm^{-1}
Frequencies
Assignments

(85008) ZEKE-PES Spectrum, Frequencies, IP

C_3H_3

(84705) Absorption Cross Sections

C_3H_4Cl
$C_3H_4ClO_2$

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$C_3H_4F_2$
IR,Raman
Frequencies
Assignments

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$C_2(CN)_2^+$
C_4HCN^+
Frequency
Modulated
Absorption
Assignments
Constants

(84714) Ultraviolet Absorption Spectra

$C_5H_{11}O_2$
$C_{10}H_{21}O_2$

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C_6H_6
IR,Raman
Spectra
Frequencies
Anharmonicities
Force Field

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$C_6H_6(^1B_{2u}, ^1B_{1u}\text{-}X)$
Absorption
Spectrum
Frequencies
Simulation

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$C_6H_6(5\nu_{CH})$
Overtone
Absorption Spectrum
Calculations

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C_6H_5CHO
Absorption
Cross Sections
HCO Fragment
Yields

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$C_{10}H_8$
LIF Spectra
Jet Cooled
Collision Free
Lifetimes
Quantum Yields

84584.	Bichutskaya, E.N., A.Z. Devdariani, A.L. Zagrebin and Yu.N. Sebyakin, "Quasi-Molecular Emission and Nonadiabatic Transitions. I. Ca($4s4p\,^3P_1$, $^3P_2$) and Mg($3s3p\,^3P_1$, $^3P_2$)-He($1s^2\ ^1S_0$) Quasi-Molecules," *Opt. Spectrosc., Russia* 87, 197-202 (1999).	$Ca(^3P_{1,2})$.He $Mg(^3P_{1,2})$.He Collision Induced Forbidden Emission Transitions
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(85013)	Photoionization Spectrum, ΔH_f, IP	*t*-HOCO

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HONO
DONO
UV Absorption
Cross Sections

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HNO_3, H_2SO_4
Aqueous Films
FTIR Spectra
Mixtures

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$HOCl(6\nu_{OH})$
Overtone Spectra
Band Origins
Erratum

(84317) Rotational Perturbations

H_2(GK-B)

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$Hg(6^3P_2\text{-}6^1S_0)$
Ne,Ar Effects
Emission,Absorption
Spectra

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$Hg(6^3P_2\text{-}6^1S_0)$
Collision Induced
Absorption
Kr,Xe Effects
Calculations

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$KrXe^+(C,B,A,X)$
PES
Spectral Constants
P.E. Curves

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MgOH,MgOD(ν_2)
Rotational
Spectra
Geometry
Constants

(84556) Chemiluminescent Spectra, $Mn+O_3$

MnO(A-X)

(84771) Absorption Coefficients, Shock Tube Measurements

NH_2,597.4 nm

(85017) Double Resonance Rydberg State Spectra, Autoionization

NH_3

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NO(C-X),(1,0)
Absorption
Cross Sections
Linestrengths
Spectral Constants

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NO_2
PFI-ZEKE Spectra
$NO_2^+(X)$
Low-lying Excited States
Constants,Energies

(84629) LIF Spectra, Radiative Lifetimes, Calculations`

$NO_2(^2B_2)$

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$N_2^+(A-X)$
(10,5),(5,1) Bands
Absorption
Cavity Ringdown
Constants

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Na_2
fs Pump/Probe
Wavepacket
PES Monitor
Laser Field Effects

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$O_2(B-X)$
Absorption Spectrum
Calculations
Comments

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Reply

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O_2
SR Continuum
Total/Partial
Absorption
Cross Sections
Predissociation
Channels

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$O_2^+(A,v=0\text{-}12)/O_2(X)$
PFI/PE Spectra
$O_2^+(A)$ Constants

84607. Song, Y., M. Evans, C.Y. Ng, C.-W. Hsu and G.K. Jarvis, "Rotationally Resolved Pulsed Field Ionization Photoelectron Bands for $O_2^+(a^4\Pi_u, v^+=0\text{-}18)$ in the Energy Range of 16.0-18.0 eV," *J. Chem. Phys.* 112, 1306-1315 (2000).

$O_2^+(a,v=0\text{-}18)/O_2(X)$
PFI/PE Spectra
$O_2^+(a)$ Constants

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O_2^+/O_2 (a)
Photoionization
Photoelectron
Distribution

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OsN,OsN_2
RuN,RuN_2
FTIR Spectra
Assignments
Frequencies
Matrix Study

(85022) Photoelectron Spectra, PO_3(A,X) Frequencies, Energies, EA(PO_3)

PO_3^-

84610. Beaton, S.A., and T.C. Steimle, "Laser Induced Fluorescence and Optical/Stark Spectroscopy of PtC," *J. Chem. Phys.* 111, 10876-10882 (1999).

PtC(A″,A′-X)
LIF,Stark
Spectra
Dipole Moments
Constants

84611. Shim, I., and K.A. Gingerich, "All-Electron ab Initio Investigations of the Three Lowest-lying Electronic States of the RuC Molecule," *Chem. Phys. Lett.* 317, 338-345 (2000).

$RuC(^1\Delta,^3\Delta,^1\Sigma^+)$
3 Low-lying States
Spectral Constants
Energies
Calculations

84612. Zen, C.-C., I.-C. Chen, Y.-P. Lee and A.J. Merer, "Laser Induced Phosphorescence of SO_2 in Solid Neon: Direct Observation of the b^3A_2 State in the $^{16}OS^{18}O$ Molecule," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 771-776 (2000).

SO_2(b,a-X)
Phosphorescence
Frequencies
Matrix Study

84613. Xue, B., Y. Chen and H.-L. Dai, "Observation of the Singlet-Triplet Pair of the 4p Rydberg State and Assignment of the Rydberg Series of SO_2," *J. Chem. Phys.* 112, 2210-2217 (2000).

SO_2
Rydberg States
Assignments

(85024) Photoelectron Spectra, EAs, Geometries, Measurements, Calculations

SO_4^-,HSO_4^-

84614. Lin, W., C.J. Evans and M.C.L. Gerry, "The Pure Rotational Spectrum of ScBr," *Phys. Chem. Chem. Phys.* 2, 43-46 (2000).

ScBr
Rotational
Spectrum
Constants
D_e

84615. Wang, X.-F., M.-H. Chen, L.-N. Zhang and Q.-Z. Qin, "Spectroscopic and Theoretical Studies on the Reactions of Laser Ablated Tantalum with Carbon Dioxide," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 758-764 (2000).

$Ta(O)CO,Ta(O)CO^-$
$Ta(O_2)(CO)_2$
FTIR Spectra
Matrix Study
Laser Ablation

(85025) Photoelectron Spectra, EAs

ZrO^-,ZrO_2^-

27. EXCITED STATE LIFETIMES/QUENCHING

(See also Section 45 for Vibrational and Rotational Relaxation Processes)

(84403)	Penning Ionization, Orientation Dependence	$Ar(^3P)+CH_3Cl$
84616.	Gonzalez-Lezana, T., M.I. Hernandez, G. Delgado-Barrio and P. Villarreal, "An Adiabatic Model for Rare Gas-Halogen van der Waals Complexes: Application to $HeBr_2(B)$," *J. Mol. Struct.* 433, 107-111 (1998).	Br_2.He(B,v) Bound States Predissociation Calculations
84617.	Stephenson, T.A., and N. Halberstadt, "Quantum Calculations on the Vibrational Predissociation of $NeBr_2$: Evidence for Continuum Resonances," *J. Chem. Phys.* 112, 2265-2273 (2000).	$Br_2(B).Ne,v\leq 20$ Vibrational Predissociation Lifetimes Dynamics Calculations
(84980)	Rotational Energy Transfer, Rate Constants	$CN(A,v=3,J)+Ar$
(84897)	Lifetimes, P.E. Curves, Low-lying States, Transition Moments, Calculations	$CO^+(B,A)$
(84583)	Lifetimes, LIF Spectra, Jet Cooled, Collision Free, Quantum Yields	$C_{10}H_8$*
84618.	Pranszke, B., P. Kierzkowski and A. Kowalski, "Electronic Branching Ratios in Chemiluminescence from the Collisions of $Ca(^3P_J,^1D_2)$ Atoms with Halogenated Methanes $CX_{4-n}Y_n(X,Y=F,Cl,Br)$," *Chem. Phys. Lett.* 317, 220-226 (2000).	$Ca(^1D,^3P)+CX_{4-n}Y_n$ Cross Sections CaX(B,A-X) Chemiluminescence Photon Yields
(84816)	Chemiluminescence, CaCl(A), CaBr(B,A) Products, Cross Section Dependences, Reaction Dynamics	$Ca(^1D_2)+HCl$ $Ca(^1D_2)+HBr$
(84584)	Collision Induced Forbidden Emission Transitions, Calculations	$Ca(^3P_{1,2})$.He $Mg(^3P_{1,2})$.He
(84585)	Collision Induced Emission Transitions, Calculations	$Ca(^1P)$.He $Ca(^1D)$.He
(84901)	Predissociation Mechanisms, P.E. Curves, Low-lying States, Calculations	ClO(A)
(84903)	Lifetimes, P.E. Curves, Spectral Constants, Low-lying States, Calculations	GaI(B,A)
(84904)	Lifetimes of 7 Low-lying Excited States, P.E. Curves, Spectral Constants, Transition Strengths, $D_e(X)$, Calculations	GaP*
(84906)	Predissociation Linewidths, P.E. Curves, Rydberg States, Calculations	$HCl(D^1\Pi,d^3\Pi)$ $DCl(D^1\Pi,d^3\Pi)$

(84642)	Lifetimes, v,J Transitions, Einstein A-Factors	H_2^+(A)
84619.	Kishimoto, N., Y. Osada and K. Ohno, "Penning Ionization of $(NH_2)_2C=X$ (X=O,S) with He(2^3S) Metastable Atoms: Difference of Anisotropic Interaction around N, O and S Atoms," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1393-1399 (2000).	He(2^3S) + $CO(NH_2)_2$ He(2^3S) + $CS(NH_2)_2$ Penning Ionization P.E. Surface Calculations PES Assignments
84620.	Skoblo, Yu.E., and V.A. Ivanov, "Role of Metastable Atoms and Molecules of Helium in Excitation Transfer to Hydrogen Atoms," *Opt. Spectrosc., Russia* 88, 151-157 (2000).	He(2^3S_1) + H_2 $He_2(^3\Sigma_u^+)$ + H_2 H(n=3-6) Product Channels Efficiencies
84621.	Browaeys, A., J. Poupard, A. Robert, S. Nowak, W. Rooijakkers, E. Arimondo, L. Marcassa, D. Boiron, C.I. Westbrook and A. Aspect," Two Body Loss Rate in a Magneto-Optical Trap of Metastable He," *Eur. Phys. J. D* 8, 199-203 (2000).	He(2^3S,2^3P) + He(2^3S) Rate Constant Ionization
84622.	Kartoshkin, V.A., "Chemi-ionization and Spin Exchange in Collisions of Excited Metastable Helium Atoms with Sodium Atoms in the Ground State: I. Kinetics of Optical Orientation," *Opt. Spectrosc., Russia* 85, 28-32 (1998).	He(2^3S_1) + Na Chemi-ionization Orientation Alignment Considerations
84623.	Kartoshkin, V.A., "Chemi-ionization and Spin Exchange in Collisions of Excited Metastable Helium Atoms with Sodium Atoms in the Ground State: II. The Calculation of Cross Sections for Chemi-ionization and Spin Exchange," *Opt. Spectrosc., Russia* 85, 177-180 (1998).	He(2^3S_1) + Na Chemi-ionization Spin Exchange Cross Sections Calculations
(84595) (84596)	Forbidden Transitions, Ne, Ar, Kr, Xe Collisional Effects	Hg(6^3P_2-6^1S_0)
84624.	Legay-Sommaire, N., and F. Legay, "Photochemical Insertion of Hg in the HCl Bond and Mercury-Sensitized Production of $ClHCl^-$ and $KrHKr^+$ in Low Temperature Matrices," *Chem. Phys. Lett.* 314, 40-46 (1999).	Hg($^3P_1$) + HCl Matrix Study HHgCl Product
84625.	Chiappero, M.S., and G.A. Arguello, "Deactivation of I($^2P_{1/2}$) by CH_3Cl, CH_2Cl_2, $CHCl_3$, CCl_3F and CCl_4," *Int. J. Chem. Kinet.* 30, 799-803 (1998).	I($^2P_{1/2}$) + M Quenching Rate Constants 5 Chloro-organics
84626.	Labazan, I., and S. Milosevic, "Lithium Vapor Excitation at (2S→3D) Two-Photon Resonance," *Eur. Phys. J. D* 8, 41-47 (2000).	Li(3^2D,2,3^2P) Energy Pooling Cross Sections

84627. Takayanagi, T., Y. Kurosaki, K. Yokoyama, K. Sato and S. Tsunashima, "Theoretical Calculations of Thermal Rate Constants for the $N(^2D)+$Acetylene Reaction," *Chem. Phys. Lett.* 312, 503-510 (1999).

$N(^2D)+C_2H_2,C_2D_2$
VTST
Rate Constants
Nonadiabatic
Transitions
Role

84628. Hewett, K.B., G.C. Manke II, D.W. Setser and G. Brewood, "Quenching Rate Constants of $NCl(a^1\Delta)$ at Room Temperature," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 539-551 (2000).

NCl(a)+M
NF(a)+M
Quenching
Rate Constants
44 Species

(84983) Rotational Relaxation, ps DFWM, Measurements

NH(A)

(84985) Rotational State to State Energy Transfer, Measurements, Analysis

$NH_2(A)+Ar$

84629. Santoro, F., and C. Petrongolo, "Nonadiabatic Radiative Lifetimes and Fluorescence Spectra of NO_2," *J. Chem. Phys.* 111, 9651-9657 (1999).

$NO_2(^2B_2)$
Radiative
Lifetimes
LIF Spectra
Calculations

84630. Nakamura, H., and S. Kato, "State Resolved Reaction Rates of the Spin-Forbidden Predissociation of N_2O: A Quantum Dynamics Study of the Rotational Effect," *J. Chem. Phys.* 112, 1785-1796 (2000).

$N_2O(1^1A')$
Predissociation
State Resolved
Reaction Rates
J Effects

(84924) Lifetime, P.E. Curves, Low-lying $1^{1,3}\Sigma^+$, $2^1\Sigma^+$ States, Stabilities, Calculations

$Na^+.He(2^1\Sigma^+)$

(84646) Predissociation, (A-X) J-Dependent Linewidths

NaI(A)

84631. Zaitsevskii, A.V., E.A. Pazyuk and A.V. Stolyarov, "Radiative Properties of Low-lying Triplet States of the NaK Molecule," *Opt. Spectrosc., Russia* 87, 225-230 (1999).

NaK(d,c,b)
Radiative
Lifetimes
S/O Interactions
Calculations

84632. Alberti, M., J.M. Lucas, B. Brunetti, F. Pirani, M. Stramaccia, M. Rosi and F. Vecchiocattivi, "Anisotropy Effects in Methyl Chloride Ionization by Metastable Neon Atoms at Thermal Energies," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1405-1415 (2000).

$Ne(^3P_{2,0})+CH_3Cl$
Penning Ionization
$CH_3Cl^+(B,A,X)$
Product Channels
Calculations

84633. Gonzalez, M., M.P. Puyuelo, J. Hernando, R. Sayos, P.A. Enriquez, J. Guallar and I. Banos, "Influence of the Collision Energy on the $O(^1D)+RH\rightarrow OH(X^2\Pi)+R(RH=CH_4,C_2H_6,C_3H_8)$ Reaction Dynamics: A Laser Induced Fluorescence and Quasiclassical Trajectory Study," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 521-529 (2000).

$O(^1D)+CH_4,C_2H_6$
$O(^1D)+C_3H_8$
Collision Energy
Effects
Product OH(v=0,1)

(84849) Reaction Dynamics, Channels, Products, Calculations — $O(^1D_2)+HCl$

84634. Chichinin, A.I., "Isotope Effects in the Deactivation of $O(^1D)$ Atoms by XCl and XF(X=H,D)," *Chem. Phys. Lett.* 316, 425-432 (2000). — $O(^1D)+HCl,HF$ $O(^1D)+DCl,DF$ Physical,Chemical Quenching Rate Constants Isotope Effects

84635. Heard, D.E., and D.A. Henderson, "Quenching of $OH(A^2\Sigma^+,v=0)$ by Several Collision Partners between 200 and 344 K: Cross Section Measurements and Model Comparisons," *Phys. Chem. Chem. Phys.* 2, 67-72 (2000). — $OH(A,v=0)+M$ Quenching Rate Constants $M=CH_4,CO,H_2,Kr$ 200-344 K

(84605) Schumann-Runge Continuum, Total/Partial Absorption Cross Sections, Predissociation Channels — O_2*

84636. Ekers, A., M. Glodz, J. Szonert, B. Bieniak, K. Fronc and T. Radelitski, "Inelastic Cross Sections and Natural Lifetimes for the $6^2D_{3/2,5/2}$ and $8^2S_{1/2}$ States of Rb," *Eur. Phys. J. D* 8, 49-58 (2000). — $Rb(6^2D_J,8^2S_{1/2})$ Mixing,Quenching Rate Constants Lifetimes

84637. Tachikawa, H., T. Hamabayashi and M. Igarashi, "Collision Energy- and Spin-Orbit Coupling-Dependence of Quenching Probability in the Electronic Energy Transfer Reaction $S(^1D)+CO\rightarrow S(^3P)+CO(v,J)$," *J. Mol. Struct.* 453, 191-196 (1998). — $S(^1D)+CO$ Quenching Branching Ratio Probabilities Calculations

84638. Lee, S.-H., and K. Liu, "Erratum - Isotope Effects and Excitation Functions for the Reactions of $S(^1D)+H_2$, D_2 and HD [*Chem. Phys. Lett.* 290, 323 (1998)]," *ibid.* 317, 516 (2000). — $S(^1D)+H_2,HD,D_2$ Erratum

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(84762) Quenching Rate Constant, $SiH_3(CHCHCl)+h\nu$ — $HSiCl^*(v,J)+Ar$

(84858) Excited (^3P) State Insertion, Reaction Dynamics — Zn^*,Cd^*,Hg^*+CH_4 Zn^*,Cd^*,Hg^*+SiH_4

28. FRANCK-CONDON FACTORS/TRANSITION PROBABILITIES

(See also Section 27 for Lifetimes and Transition Probabilities)

(84897) Transition Moments, P.E. Curves, Lifetimes, Calculations — $CO^+(B,A-X)$

(84904) Low-lying States, Transition Strengths, Lifetimes, P.E. Curves, Spectral Constants, $D_e(X)$, Calculations — GaP*

84640. Astashkevich, S.A., and B.P. Lavrov, "Absolute Values of Rovibronic Transition Probabilities for the ($I^1\Pi_g^- \rightarrow B^1\Sigma_u^+$) System of Bands of the H_2 Molecule," *Opt. Spectrosc., Russia* 85, 348-355 (1998).

H_2(I-B)
Transition Probabilities Calculations

84641. Astashkevich, S.A., and B.P. Lavrov, "Probabilities of Spontaneous ($J^1\Delta_g^- \rightarrow B^1\Sigma_u^+$) Transitions in the H_2 Molecule Forbidden in the Adiabatic Approximation," *Opt. Spectrosc., Russia* 85, 504-509 (1998).

H_2(J-B)
Transition Probabilities

84642. Bunker, P.R., and R.E. Moss, "Forbidden Electric Dipole Rotation and Rotation-Vibration Transition in H_2^+," *Chem. Phys. Lett.* 316, 266-270 (2000).

H_2^+(A,X)
State Interactions
Einstein A-Factors
Lifetimes

(84912) Transition Moments, Two Lowest Singlet States, P.E. Surfaces

H_3^+

84643. Akopyan, M.E., T.F. Bachina, N.K. Bibinov, V.V. Grebenev, D.B. Kokh, V.A. Ozolov and A.M. Pravilov, "Dipole Moment of the ($E0_g^+$-$B0_u^+$) Transition in an Iodine Molecule," *Opt. Spectrosc., Russia* 84, 651-655 (1998).

I_2(E-B)
Dipole Moment
Internuclear Separation Dependence
Measurements

84644. Lee, P.C., and J.B. Nee, "Detection of O(^{1}D) Produced in the Photodissociation of O_2. I. Identification of the $^3\Sigma_u^-$ and $^3\Pi_u$ Rydberg States in 113-130 nm," *J. Chem. Phys.* 112, 1763-1768 (2000).

O_2(F,E-X)
113-130 nm
Oscillator Strengths
O(^{1}D) Product Quantum Yield Dependences

29. LINESHAPES/STRENGTHS

(84565) Vibrational Autoionization Linewidths

HCO
Rydberg States

(84957) Infrared Intensities, Structural Calculations, Geometries, Frequencies

FeH_3, ScH_3
TiH_3, VH_3

(84906) Predissociation Linewidths, P.E. Curves, Rydberg States, Calculations

HCl($D^1\Pi$,$d^3\Pi$)
DCl($D^1\Pi$,$d^3\Pi$)

84645. Astashkevich, S.A., M.V. Kalachev and B.P. Lavrov, "Observation of Perturbations in the Probabilities of the ($GK^1\Sigma_g^+ \rightarrow B^1\Sigma_u^+$) Spontaneous Transitions of the H_2 Molecule: Rotational Branching Ratios," *Opt. Spectrosc., Russia* 87, 212-218 (1999).

H_2(GK-B)
Linestrength Ratios
Measurements
Perturbations

(84599) Linestrengths, Absorption Cross Sections, Spectral Constants

NO(C-X),(1,0)

(84966) Infrared Intensities, Structural Calculations, Isomers, Geometries, Frequencies, Dipole Moments

N_2O_4

84646. Baba, M., T. Kokita, S. Kasahara and H. Kato, "Variation of the Linewidth of the ($A0^+ \leftarrow X^1\Sigma^+$) Transition of NaI," *J. Chem. Phys.* 111, 9574-9576 (1999).

NaI(A-X)
Excitation
J Dependent
Linewidths
Predissociation

(84318) Rotational Lineshapes, Diode Laser, Temperatures

O_2(b-X),(0,0)

84647. Franzke, J., H.D. Wizemann, K. Niemax and C. Vadla, "Impact Broadening and Shift Rates for the ($6p^2\ ^3P_{J'} \rightarrow 7s^3P_J^\circ$) Transitions of Lead Induced by Collisions with Argon and Helium," *Eur. Phys. J. D* 8, 23-28 (2000).

Pb($7^3P_{1,0}$-$6^3P_{2,1}$)
Absorption
Broadening
Coefficients

30. ANALYSIS/MONITORING TECHNIQUES

84648. Kohse-Hoinghaus, K., "Laser and Probe Diagnostics in Fundamental Combustion Research," *Isr. J. Chem.* 39, 25-39 (1999).

Laser Diagnostics
Combustion
Applications
Review

84649. Ebert, V., C. Schulz, H.-R. Volpp, J. Wolfrum and P. Monkhouse, "Laser Diagnostics of Combustion Processes: From Chemical Dynamics to Technical Devices," *Isr. J. Chem.* 39, 1-24 (1999).

Laser Diagnostics
Catalytic
Combustion
Engines
T,NO,Alkalis
Incineration
Review

84650. Hunter, A.J.R., J.R. Morency, C.L. Senior, S.J. Davis and M.E. Fraser, "Continuous Emissions Monitoring Using Spark Induced Breakdown Spectroscopy," *J. Air Waste Manage. Assoc.* 50, 111-117 (2000).

Spark Induced
Breakdown Spectra
Metal/Aerosols
Atomic Analysis
Monitoring

(84722) Photoionization Monitor

CH_2OH

84651. Li, J., V.M. Bierbaum and S.R. Leone, "Laser Ionization Time-of-Flight Mass Spectrometer Detection of Methyl Radical Produced by Ion-Molecule Reactions in a Flowing-Afterglow Apparatus," *Chem. Phys. Lett.* 313, 76-84 (1999).

Laser Ionization
TOF
CH_3
Monitor
$CO^+ + CH_4$
$N_2O^+ + CH_4$

84652. Popp, P.J., G.A. Bishop and D.H. Stedman, "Development of a High Speed Ultraviolet Spectrometer for Remote Sensing of Mobile Source Nitric Oxide Emissions," *J. Air Waste Manage. Assoc.* 49, 1463-1468 (1999).

NDUV Absorption
NO
Monitor
Automobile
Monitoring

84653. Booth, J.P., G. Cunge, L. Biennier, D. Romanini and A. Kachanov, "Ultraviolet Cavity Ringdown Spectroscopy of Free Radicals in Etching Plasmas," *Chem. Phys. Lett.* 317, 631-636 (2000).

UV Absorption
Cavity Ringdown
AlF,CF
CF_2,SiF_2
Monitor

84654. Derzy, I., V.A. Lozovsky and S. Cheskis, "CH, NH and NH_2 Concentration Profiles in Methane/Air Flames Doped with N_2O," *Isr. J. Chem.* 39, 49-54 (1999).

Absorption
Laser Intracavity
Cavity Ringdown
CH,NH,NH_2
Monitors
$CH_4/O_2/N_2$

(84663) Intracavity Absorption, CH_4/Air Flame Profile

$^1CH_2$

84655. Hippler, M., and M. Quack, "cw Cavity Ringdown Infrared Absorption Spectroscopy in Pulsed Supersonic Jets: Nitrous Oxide and Methane," *Chem. Phys. Lett.* 314, 273-281 (1999).

Absorption
Cavity Ringdown
$CH_4(\nu_2+2\nu_3)$
$N_2O(\nu_1+3\nu_3)$
Supersonic Jet
Monitor

(84573) Absorption, Cavity Ringdown Monitor

C_2H_3

(84717) Cavity Ringdown Absorption Monitor

C_6H_5

84656. King, M.D., E.M. Dick and W.R. Simpson, "A New Method for the Atmospheric Detection of the Nitrate Radical, NO_3," *Atm. Environ.* 34, 685-688 (2000).

Absorption
Cavity Ringdown
NO_3
Monitor
Sensitivity

(84661) Species Profiles, CH_4, H_2 Flames, Flame Speciation

LIF,As

84657. Crosley, D.R., J.B. Jeffries and G.P. Smith," Absolute Concentration Measurements of Chemically-Important Flame Radicals," *Isr. J. Chem.* 39, 41-48 (1999).

LIF
CH,HCO,NO,OH
$CH_4/O_2/N_2$
GRI-Mech
Kinetic Model
Validation

84658. McIlroy, A., "Laser Studies of Small Radicals in Rich Methane Flames: OH, HCO and $^1CH_2$," *Isr. J. Chem.* 39, 55-62 (1999).

LIF
Cavity Ringdown
Monitors
$^1CH_2$,HCO,OH
Rich CH_4 Flames
Kinetic Model
Adequacies

84659. Zobnin, A.V., A.P. Nefedov, V.A. Sinel'shchikov and A.D. Usachev, "Role of Photochemical Processes in the Use of Laser Induced Fluorescence at 230.1 nm for the Diagnostics of Hydrocarbon Flames," *Opt. Spectrosc., Russia* 87, 23-28 (1999).

LIF
CO
230.1 nm Perturbing Effects
CO_2(v) Absorptions

84660. Tong, X., R.B. Barat and A.T. Poulos, "Detection of Mercuric Bromide in a Gas Phase Flow Cell by Laser Photofragment Fluorescence Spectroscopy," *Environ. Sci. Technol.* 33, 3260-3263 (1999).

Photofragment Fluorescence
$HgBr_2$
Real-time Monitor
Hg(253.7 nm) Detection

31. FLAME CONCENTRATION MEASUREMENTS

(See also Section 34 for Flame Species Profiles)

84661. Zhang, Y., Y. Yoon, P.B. Kelly and I.M. Kennedy, "LIF Measurements of Atomic Arsenic in Hydrogen and Methane Diffusion Flames," *Symp. (Int.) Combust. Proc.* 27, 1777-1783 (1998).

As
Flame Speciation
CH_4,H_2 Flames
LIF Monitor
Atomic Profiles

84662. Berg, P.A., D.A. Hill, A.R. Noble, G.P. Smith, J.B. Jeffries and D.R. Crosley, "Absolute CH Concentration Measurements in Low Pressure Methane Flames: Comparisons with Model Results," *Combust. Flame* 121, 223-235 (2000).

CH
Flame Profiles
LIF,Rayleigh
$CH_4/O_2/N_2$ Flames

84663. Derzy, I., V.A. Lozovsky and S. Cheskis, "Absorption Cross Sections and Absolute Concentration of Singlet Methylene in Methane/Air Flames," *Chem. Phys. Lett.* 313, 121-128 (1999).

$^1CH_2$
Flame Profiles
Intracavity Absorption
CH_4/Air

84664. Yu, S., A.D. Jones, D.P.Y. Chang, P.B. Kelly and I.M. Kennedy, "The Transformation of Chromium in a Laminar Premixed Hydrogen/Air Flame," *Symp. (Int.) Combust. Proc.* 27, 1639-1645 (1998).

Cr
Flame Speciation
H_2/Air
Probe Sampling
Kinetic Model

32. MAPPING/TOMOGRAPHIC METHODS

(84279) Spray Flame Visualization, CH*, OH* Spectral Emission, Cluster Disappearance

Laser Tomography

(84432) 2-D Mapping, I.C. Engine, DI Gasoline

LIF,$(CH_3)_2CO$ Tracer

(84445) In-Cylinder Planar Measurements, I.C. Engine, Equivalence Ratio Effects

PLIF,NO

(84767) 2-D Mapping, Product Orientation, OCS + hν — $S(^1D_2)$

33. OPTOGALVANIC/OPTOACOUSTIC METHODS

34. FLAME KINETIC MODELING

84665. Held, T.J., and F.L. Dryer, "A Comprehensive Mechanism for Methanol Oxidation," *Int. J. Chem. Kinet.* 30, 805-830 (1998). — Kinetic Modeling; CH_3OH/O_2; Comprehensive Mechanism; Various Data Sets

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(84357) Reduced Kinetic Models, Ramjet Combustion — $CH_4, H_2/O_2$

(84658) $^1CH_2$, HCO, OH Species Profiles, LIF and Cavity Ringdown Monitoring, Kinetic Model Adequacies — Rich CH_4 Flames

84667. Al-Farayedhi, A.A., M.A. Antar and A. Khan, "Effect of the Equivalence Ratio on the Concentration of $CH_4/NO_2/O_2$ Combustion Products," *Int. J. Energy Res.* 23, 1165-1175 (1999). — Kinetic Modeling; $CH_4/NO_2/O_2$; Species Profiles; Data Comparisons

(84511) NO Formation, Simplified Kinetic Model, Adequacies — CH_4/Air

(84657) CH, HCO, NO, OH Species Profiles, LIF Monitor, GRI-Mech Kinetic Model Adequacies — $CH_4/O_2/N_2$

(84654) CH, NH, NH_2 Species Profiles, Cavity Ringdown Monitor, GRI-Mech Kinetic Model Adequacies — $CH_4/O_2/N_2$

84668. Crunelle, B., A. Turbiez and J.-F. Pauwels, "Chemical Structure of Methane and Ethane Flames," *J. de Chim. Phys.* 96 1146-1171 (1999). — Kinetic Modeling; $CH_4/O_2/Ar$; $C_2H_6/O_2/Ar$; Species Profiles Measurements

84669. Fournet, R., J.C. Bauge and F. Battin-Leclerc, "Experimental and Modeling of Oxidation of Acetylene, Propyne, Allene and 1,3-Butadiene," *Int. J. Chem. Kinet.* 31, 361-379 (1999). — Kinetic Modeling; $C_2H_2/O_2/Ar$; $C_3H_4/O_2/Ar$; $C_4H_6/O_2/Ar$; Shock Tube Ignition Delays

84670. Marinov, N.M., "A Detailed Chemical Kinetic Model for High Temperature Ethanol Oxidation," *Int. J. Chem. Kinet.* 31, 183-220 (1999).

Kinetic Modeling
C_2H_5OH/O_2
Data Set Fitting
$C_2H_5OH + M$
Rate Constants

84671. D'Anna, A., A. Violi and A. D'Alessio, "Modeling the Rich Combustion of Aliphatic Hydrocarbons," *Combust. Flame* 121, 418-429 (2000).

Kinetic Modeling
Rich Aliphatic Flames
C_6H_6,PAH
Formation Profiles

84672. Bauge, J.C., F. Battin-Leclerc and F. Baronnet, "Experimental and Modeling Study of the Oxidation of Isobutene," *Int. J. Chem. Kinet.* 30, 629-640 (1998).

Kinetic Modeling
i-C_4H_8/O_2
Stirred Reactor
i-$C_4H_8/O_2/Ar$
Shock Tube
Ignition Delays
Mechanism

84673. Glaude, P.A., V. Warth, R. Fournet, F. Battin-Leclerc, G. Scacchi and G.M. Come, "Modeling of the Oxidation of *n*-Octane and *n*-Decane Using an Automatic Generation of Mechanisms," *Int. J. Chem. Kinet.* 30, 949-959 (1998).

Kinetic Modeling
n-C_8H_{18}/O_2
n-$C_{10}H_{22}/O_2$
Software Generated Mechanism
Data Comparisons

84674. Tonse, S.R., N.W. Moriarty, N.J. Brown and M. Frenklach, "PRISM: Piecewise Reusable Implementation of Solution Mapping: An Economical Strategy for Chemical Kinetics," *Isr. J. Chem.* 39, 97-106 (1999).

Kinetic Modeling
$H_2/Air/N_2$
Hypercube Piecemeal Solving Method

84675. Mueller, M.A., T.J. Kim, R.A. Yetter and F.L. Dryer, "Flow Reactor Studies and Kinetic Modeling of the H_2/O_2 Reaction," *Int. J. Chem. Kinet.* 31, 113-125 (1999).

Kinetic Modeling
H_2/O_2
T,H_2,O_2,H_2O
Species Profiles
Flow Reactor

84676. Mueller, M.A., R.A. Yetter and F.L. Dryer, "Flow Reactor Studies and Kinetic Modeling of the $H_2/O_2/NO_x$ and $CO/H_2O/O_2/NO_x$ Reactions," *Int. J. Chem. Kinet.* 31, 705-724 (1999).

Kinetic Modeling
$H_2/O_2(NO,NO_2)$
$CO/H_2O/O_2(NO,NO_2)$
Flow Reactor
Species Profiles
Adequacies

35. PYROLYSIS KINETICS/STUDIES

(See also Section 4 for Coal Pyrolysis)

84677.	Gupta, A.K., and P. Muller, "Pyrolysis of Paper and Cardboard in Inert and Oxidative Environments," Presented Originally as AIAA Paper 98-0264 at the *36th AIAA Aerospace Sciences Meeting*, Held in Reno NV, January 1998, *J. Propulsion Power* 15, 187-194 (1999).	Pyrolysis Paper,Cardboard Thermogravimetric Analysis Kinetics Char Yields
(84486)	Pyrolysis, Destructive Efficiencies, Products	$CBrF_3/H_2$
(84534)	Soot Formation, Kinetic Model Adequacies	Pyrolysis Hydrocarbons
84678.	Zhang, Y.-X., and S.H. Bauer, "Gas Phase Decomposition Mechanisms of C-NO_2, N-NO_2 Energetic Materials: Reevaluations," *Int. J. Chem. Kinet.* 31, 655-673 (1999).	Pyrolysis CH_3NO_2,CH_3ONO $(CH_3)_2NNH_2$,TNAZ Fragmentation Mechanisms
84679.	Salouhi, M., P.M. Marquaire and G.M. Come, "Pyrolysis of 1,2-Dichloroethane at About 500 °C," *J. de Chim. Phys.* 96, 797-809 (1999).	Pyrolysis $C_2H_4Cl_2$ Stirred Reactor Homogeneous/ Heterogeneous Mechanism
84680.	Zhang, Y.-X., and S.H. Bauer, "The Gas Phase Pyrolysis of 2,2-Dinitropropane: Shock Tube Kinetics," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1217-1225 (2000).	Pyrolysis $C_3H_6(NO_2)_2$/Ar Rate Constants T Dependence Kinetic Model Shock Tube Products
84681.	Zhang, Y.-X., and S.H. Bauer, "Gas Phase Pyrolyses of 2-Nitropropane and 2-Nitropropanol: Shock Tube Kinetics," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1207-1216 (2000).	Pyrolysis $C_3H_7NO_2$/Ar *i*-$C_3H_6(OH)NO_2$/Ar Rate Constants Shock Tube
84682.	Zils, R., D. Perrin and R. Martin, "Kinetic Study and Modeling of the Hetero-, Homogeneous Pyrolysis and Oxidation of Isobutane Around 800 K. III. Pyrolysis-Oxidation in Unpacked and in PbO Coated Packed Pyrex Reactors," *Int. J. Chem. Kinet.* 30, 657-671 (1998).	Pyrolysis *i*-C_4H_{10} *i*-C_4H_{10}/O_2 Mechanisms Modeling

84683. Brioukov, M.G., J. Park and M.C. Lin, "Kinetic Modeling of Benzene Decomposition Near 1000 K: The Effects of Toluene Impurity," *Int. J. Chem. Kinet.* 31, 577-582 (1999).
Pyrolysis
C_6H_6
Kinetic Modeling
$C_6H_5CH_3$ Impurity Effects

84684. Chuchani, G., and R.M. Dominguez, "Kinetics of the Gas Phase Elimination of α-Bromophenylacetic Acid under Maximum Inhibition," *Int. J. Chem. Kinet.* 31, 725-728 (1999).
Pyrolysis
$C_6H_5CH_2BrCOOH$
Elimination
Mechanism
Products

(84550) Pyrolysis, C_n Nanotubes Formation
$Fe(CO)_5/CO$

(84537) Pyrolysis, PbO Particle Formation
$Pb(NO_3)_2$ Spray

(84536) Pyrolysis, Product Particle Formation, PbO, $Ni(OH)_2$
$Pb(NO_3)_2$ Droplets
$Ni(NO_3)_2$ Droplets

36. KINETIC MODELING/SENSITIVITIES/RATE CONSTANTS

(See also Section 15 for Ion Reaction Rate Constants, Section 27 for Excited State Rate Constants, Section 35 for Pyrolysis Rate Constants, Section 39 for Unimolecular Rate Constants, Section 40 for Theoretically Calculated Values and Section 45 for Energy Relaxation Rate Constants)

(84763) Infrared Chemiluminescence Measuring Method, Reaction Products, Sensitivities, Review
Rate Constants

84685. Bedjanian, Y., G. Poulet and G. Le Bras, "Low-Pressure Study of the Reactions of Br Atoms with Alkenes. III. Reactions with 2-Methyl-2-butene, 2,3-Dimethyl-2-butene, and 1-Hexene," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 577-583 (2000).
$Br+C_5H_{10}$
$Br+C_6H_{12}$
Rate Constants
T Dependences
$\Delta H_f(C_5H_{10}Br,C_6H_{12}Br)$

84686. Bedjanian, Y., G. Le Bras and G. Poulet, "Kinetic Study of the Reactions $Br+IBr \rightarrow I+Br_2$ and $I+Br_2 \rightarrow Br+IBr$," *Int. J. Chem. Kinet.* 30, 933-940 (1998).
$Br+IBr$
$I+Br_2$
Rate Constants
$\Delta H_{Reaction}, \Delta H_f(IBr)$

84687. Bedjanian, Y., G. Le Bras and G. Poulet, "Kinetic Study of the Reactions of Br_2 with OH and OD," *Int. J. Chem. Kinet.* 31, 698-704 (1999).
Br_2+OH
Br_2+OD
Rate Constants
T Dependences
Channels

84688. Smith, S.R., and B.E. Holmes, "Substituent Effects on the Disproportionation-Combination Rate Constant Ratios for Gas Phase Halocarbon Radicals. IV. Reactions of $CF_3+CF_3CH_2CF_2$ and $CF_3CH_2CF_2+CF_3CH_2CF_2$," *Int. J. Chem. Kinet.* 31, 237-243 (1999).
$CF_3+CF_3CH_2CF_2$
$CF_3CH_2CF_2+CF_3CH_2CF_2$
Rate Constant Ratios

84689. Biggs, P., C.E. Canosa-Mas, C.J. Percival, D.E. Shallcross and R.P. Wayne, "A Study of the Self Reaction of CH_2ClO_2 and $CHCl_2O_2$ Radicals at 298 K," *Int. J. Chem. Kinet.* 31, 433-444 (1999).

$CHCl_2O_2 + CHCl_2O_2$
$CH_2ClO_2 + CH_2ClO_2$
$CH_3O_2 + CH_3O_2$
Rate Constants

84690. Glarborg, P., A.B. Bendtsen and J.A. Miller, "Nitromethane Dissociation: Implications for the $CH_3 + NO_2$ Reaction," *Int. J. Chem. Kinet.* 31, 591-602 (1999).

$CH_3 + NO_2$
Rate Constant
$S_{298}(CH_3NO_2)$
Assessments

84691. Wallington, T.J., O.J. Nielsen and K. Sehested, "Kinetics of the Reaction of CH_3O_2 Radicals with NO_2," *Chem. Phys. Lett.* 313, 456-460 (1999).

$CH_3O_2 + NO_2(+M)$
Rate Constants
Fall-off Parameters

84692. Sokolov, O., M.D. Hurley, J.C. Ball, T.J. Wallington, W. Nelson, I. Barnes and K.H. Becker, "Kinetics of the Reactions of Chlorine Atoms with CH_3ONO and CH_3ONO_2," *Int. J. Chem. Kinet.* 31, 357-359 (1999).

$CH_3ONO + Cl$
$CH_3ONO_2 + Cl$
Rate Constants

84693. Kukui, A., V. Bossoutrot, G. Laverdet and G. Le Bras, "Mechanism of the Reaction of CH_3SO with NO_2 in Relation to Atmospheric Oxidation of Dimethyl Sulfide: Experimental and Theoretical Study," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 935-946 (2000).

$CH_3SO + NO_2$
$CH_3SO_2 \rightarrow$
Rate Constants
Mechanisms

84694. Ochimizu, T., K. Seki, M. Yagi, J.B. Halpern and H. Okabe, "Rate Constants for the Reactions of CN with C_6-C_8 Unsaturated Hydrocarbons: The Relations between the Reaction Rates and the Molecular Lengths," *Chem. Phys. Lett.* 313, 451-455 (1999).

$CN + C_6H_8$
$CN + C_8H_{10}$
Rate Constants
Measurements

84695. Kruse, T., and P. Roth, "High Temperature Reaction of C_2 with NO Including Product Channel Measurements," *Int. J. Chem. Kinet.* 31, 11-21 (1999).

$C_2 + NO$
Rate Constants
T Dependence
Product Channels
Branching Ratios

84696. Teruel, M.A., R.A. Taccone and S.I. Lane, "Discharge Flow-Chemiluminescence Study of the Rate Coefficients for $O(^3P) + CF_2=CCl_2$ and $O(^3P) + CF_3CF=CF_2$ Reactions at 298 K," *Int. J. Chem. Kinet.* 31, 867-872 (1999).

$CF_2CCl_2 + O$
$C_3F_6 + O$
Rate Constants

84697. Wallington, T.J., and E.W. Kaiser, "Comment on The Fluorine Atom Initiated Oxidation of CF_3CFH_2(HFC-134a) Studied by FTIR Spectroscopy by A.S. Hasson, et al.," *Int. J. Chem. Kinet.* 31, 397-398 (1999).

$CF_3CFHO + O_2$
$CF_3CFHO + M$
Rate Constants
Comments

84698. Hasson, A.S., C.M. Moore and I.W.M. Smith, "Response to a Comment by T.J. Wallington and E.W. Kaiser on The Fluorine Atom Initiated Oxidation of CF_3CFH_2(HFC-134a) Studied by FTIR Spectroscopy by A.S. Hasson, et al.," *Int. J. Chem. Kinet.* 31, 399-400 (1999).

Reply

84699. Rim, K.T., and J.F. Hershberger, "Product Branching Ratio of the HCCO+NO Reaction," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 293-296 (2000).

HCCO+NO
Channels
Branching Ratios
$CH_2CO+h\nu(193\ nm)$
Quantum Yields

84700. Sehested, J., L.K. Christensen, O.J. Nielsen and T.J. Wallington, "Absolute Rate Constants for $F+CH_3CHO$ and CH_3CO+O_2, Relative Rate Study of CH_3CO+NO, and the Production Distribution of the $F+CH_3CHO$ Reaction," *Int. J. Chem. Kinet.* 30, 913-921 (1998).

CH_3CHO+F
Rate Constant
Product Yields
CH_3CO,CH_2CHO
CH_3CO+NO,O_2
Rate Constants

84701. Fittschen, C., A. Frenzel, K. Imrik and P. Devolder, "Rate Constants for the Reactions of C_2H_5O, *i*-C_3H_7O, and *n*-C_3H_7O with NO and O_2 as a Function of Temperature," *Int. J. Chem. Kinet.* 31, 860-866 (1999).

C_2H_5O+NO,O_2
C_3H_7O+NO,O_2
Rate Constants
T Dependences

(84670) Rate Constants, C_2H_5OH/O_2 Constant Volume Bomb and Counterflow Twin Flame Data, Kinetic Modeling Fit

C_2H_5OH+M

84702. Alzueta, M.U., J. Muro, R. Bilbao and P. Glarborg, "Oxidation of Dimethyl Ether and Its Interaction with Nitrogen Oxides," *Isr. J. Chem.* 39, 73-86 (1999).

Kinetic Modeling
$(CH_3)_2O/O_2$
Flow Reactor
NO,NO_2 Additive Effects

84703. Maurer, T., I. Barnes and K.H. Becker, "FTIR Kinetic and Product Study of the Br-Initiated Oxidation of Dimethyl Sulfide," *Int. J. Chem. Kinet.* 31, 883-893 (1999).

$(CH_3)_2S+Br$
Rate Constant
Major Sulfur Products

84704. Tokuhashi, K., A. Takahashi, M. Kaise, S. Kondo, A. Sekiya, S. Yamashita and H. Ito, "Rate Constants for the Reactions of OH Radicals with $CH_3OCF_2CF_3$, $CH_3OCF_2CF_2CF_3$ and $CH_3OCF(CF_3)_2$," *Int. J. Chem. Kinet.* 31, 846-853 (1999).

$C_2F_5OCH_3+OH$
$C_3F_7OCH_3+OH$
Rate Constants
T Dependences

84705. Atkinson, D.B., and J.W. Hudgens, "Chlorination Chemistry. II. Rate Coefficients, Reaction Mechanism and Spectrum of the Chlorine Adduct of Allene," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 811-818 (2000).

$C_3H_4+Cl(+M)$
$C_3H_4Cl+C_3H_4Cl$
$C_3H_4Cl+O_2$
Rate Constants
C_3H_4Cl
$C_3H_4ClO_2$
Absorption Cross Sections

84706. Roden, P.J., M.S. Stark and D.J. Waddington, "The Reaction of Acrolein with Acetylperoxyl Radicals in the Gas Phase," *Int. J. Chem. Kinet.* 31, 277-282 (1999).

$C_2H_3CHO+CH_3C(O)O_2$
Rate Constant

84707. Tokuhashi, K., A. Takahashi, M. Kaise, S. Kondo, A. Sekiya, S. Yamashita and H. Ito, "Rate Constants for the Reactions of OH Radicals with $CH_3OCF_2CHF_2$, $CHF_2OCH_2CF_2CHF_2$, $CHF_2OCH_2CF_2CF_3$ and $CF_3CH_2OCF_2CHF_2$ over the Temperature Range 250-430 K," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1165-1170 (2000).

$CH_3OC_2HF_4+OH$
$CHF_2OC_3H_3F_4+OH$
$CHF_2OC_3H_2F_5+OH$
$CF_3CH_2OC_2HF_4+OH$
Rate Constants
T Dependences

84708. Froyd, K.D., and E.R. Lovejoy, "Direct Measurement of the $C_2H_5C(O)O_2+NO$ Reaction Rate Coefficient Using Chemical Ionization Mass Spectrometry," *Int. J. Chem. Kinet.* 31, 221-228 (1999).

$C_2H_5C(O)O_2+NO$
Rate Constants
T Dependence
Measurements

84709. Meinike, T., L. Engelmann, M. Olzmann and K. Scherzer, "Rate Coefficients for the Reactions of Hydrogen Atoms with 1-Bromopropane, 2-Bromopropane, 1-Bromobutane and 2-Bromobutane," *Int. J. Chem. Kinet.* 30, 721-727 (1998).

C_3H_7Br+H
C_4H_9Br+H
Rate Constants

84710. Thuner, L.P., I. Barnes, T. Maurer, C.G. Sauer and K.H. Becker, "Kinetic Study of the Reaction of OH with a Series of Acetals at 298(±4) K," *Int. J. Chem. Kinet.* 31, 797-803 (1999).

$CH_2(OR)_2+OH$
$R=C_1$-C_4 Alkyl
Rate Constants

84711. Kramp, F., and S.E. Paulson, "The Gas Phase Reaction of Ozone with 1,3-Butadiene: Formation Yields of Some Toxic Products," *Atm. Environ.* 34, 35-43 (2000).

$C_4H_6+O_3$
Organics,OH
Product Yields
$C_4H_6O+O_3$
Rate Constant

84712. Stevens, P., D. L'Esperance, B. Chuong and G. Martin, "Measurements of the Kinetics of the OH Initiated Oxidation of Isoprene: Radical Propagation in the OH+Isoprene+O_2+NO Reaction System," *Int. J. Chem. Kinet.* 31, 637-643 (1999).

C_5H_8+OH
Rate Constant
C_5H_8/OH/NO/O_2
Mechanism

84713. Wyatt, S.E., J.S. Baxley and J.R. Wells, "The Hydroxyl Radical Reaction Rate Constant and Products of Methyl Isobutyrate," *Int. J. Chem. Kinet.* 31, 551-557 (1999).

$C_3H_7COOCH_3+OH$
Rate Constant
Product Yields

84714. Boyd, A.A., E. Villenave and R. Lesclaux, "Structure-Reactivity Relationships for the Self-Reactions of Linear Secondary Alkylperoxy Radicals: An Experimental Investigation," *Int. J. Chem. Kinet.* 31, 37-46 (1999).

$C_5H_{11}O_2+C_5H_{11}O_2$
$C_{10}H_{21}O_2+C_{10}H_{21}O_2$
Rate Constants
UV Absorption
Spectra

84715. Markgraf, S.J., J. Semples and J.R. Wells, "The Hydroxyl Radical Reaction Rate Constant and Atmospheric Transformation Products of 2-Propoxyethanol," *Int. J. Chem. Kinet.* 31, 315-322 (1999).

$C_3H_7OC_2H_4OH+OH$
Rate Constant
Product Yields
Atmospheric
Lifetime

84716. Nam, G.-J., W. Xia, J. Park and M.C. Lin, "The Reaction of C_6H_5 with CO: Kinetic Measurement and Theoretical Correlation with the Reverse Process," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1233-1239 (2000).

$C_6H_5+CO+Ar$
Rate Constants
RRKM Analysis
$\Delta H_f(C_6H_5CO)$

84717. Park, J., S.I. Gheyas and M.C. Lin, "Kinetics of C_6H_5 Radical Reactions with 2-Methylpropane, 2,3-Dimethylbutane and 2,3,4-Trimethylpentane," *Int. J. Chem. Kinet.* 31, 645-653 (1999).

$C_6H_5 + t\text{-}C_4H_{10}$
$C_6H_5 + ((CH_3)_2CH)_2$
$C_6H_5 + ((CH_3)_2CH)_2CH(CH_3)$
Rate Constants
Cavity Ringdown
Absorption

84718. Tao, Z., and Z. Li, "A Kinetics Study on Reactions of C_6H_5O with C_6H_5O and O_3 at 298 K," *Int. J. Chem. Kinet.* 31, 65-72 (1999).

$C_6H_5O + C_6H_5O$
$C_6H_5O + O_3$
Rate Constants
Products

84719. Harry, C., J. Arey and R. Atkinson, "Rate Constants for the Reactions of OH Radicals and Cl Atoms with Di-*n*-Propyl Ether and Di-*n*-Butyl Ether and Their Deuterated Analogs," *Int. J. Chem. Kinet.* 31, 425-431 (1999).

$(C_3H_7)_2O + Cl,OH$
$(C_4H_9)_2O + Cl,OH$
D-Analogs
Rate Constants
Measurements

84720. Klotz, B., I. Barnes, B.T. Golding and K.-H. Becker, "Atmospheric Chemistry of Toluene-1,2-oxide/2-methyloxepin," *Phys. Chem. Chem. Phys.* 2, 227-235 (2000).

$c\text{-}C_6H_5O(CH_3) + M$
$M = OH, NO_3, h\nu$
Rate Constants
Isomers

84721. Orlando, J.J., "Temperature Dependence of the Rate Coefficients for the Reaction of Chlorine Atoms with Chloromethanes," *Int. J. Chem. Kinet.* 31, 515-524 (1999).

$Cl + CH_3Cl$
$Cl + CH_2Cl_2, CHCl_3$
$Cl + HCOCl$
Rate Constants
T Dependences
CH_2Cl_2/O_2
Oxidation Mechanism

84722. Ahmed, M., D.S. Peterka and A.G. Suits, "H Absorption Dynamics by Crossed Beam Velocity Map Imaging: $Cl + CH_3OH \rightarrow CH_2OH + HCl$," *Chem. Phys. Lett.* 317, 264-268 (2000).

$Cl + CH_3OH$
Cross Sections
CH_2OH Product
Photoionization
Monitor

84723. Tyndall, G.S., J.J. Orlando, C.S. Kegley-Owen, T.J. Wallington and M.D. Hurley, "Rate Coefficients for the Reactions of Chlorine Atoms with Methanol and Acetaldehyde," *Int. J. Chem. Kinet.* 31, 776-784 (1999).

$Cl + CH_3OH, CH_2OH$
$Cl + CH_3CHO, CH_3CO$
$CH_3CO + O_2$
Rate Constants

84724. Mauer, T., T.J. Wallington, I. Barnes and K.H. Becker, "Kinetics of the Gas Phase Reaction of Cl Atoms with $CF_2ClCFClH$ at 263-313 K," *Int. J. Chem. Kinet.* 31, 785-788 (1999).

$Cl + CF_2ClCHFCl$
Rate Constants
T Dependence

84725. Kegley-Owen, C.S., G.S. Tyndall, J.J. Orlando and A. Fried, "Tunable Diode Laser Studies of the Reaction of Cl Atoms with CH_3CHO," *Int. J. Chem. Kinet.* 31, 766-775 (1999).

$Cl + CH_3CHO$
Rate Constant
HCl(v) Product Distributions
$HCl(v=1) + CH_3CHO$ Quenching Rate Constant

84726. Christensen, L.K., J.C. Ball and T.J. Wallington, "Atmospheric Oxidation Mechanism of Methyl Acetate," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 345-351 (2000).

$Cl + CH_3COOCH_3$
$Cl + CH_3COCH_3$
$Cl + CH_3COOCHO$
$Cl + ClCH_2COOCH_3$
Rate Constants
Channels

84727. Kandel, S.A., A.J. Alexander, Z.H. Kim, R.N. Zare, F.J. Aoiz, L. Banares, J.F. Castillo and V.S. Rabanos, "Cl + HD(v=1;J=1,2) Reaction Dynamics: Comparison between Theory and Experiment," *J. Chem. Phys.* 112, 670-685 (2000).

$Cl + HD(v=1,J=1,2)$
Cross Sections
Products
Data/Theory Comparisons

84728. Nickolaisen, S.L., C.M. Roehl, L.K. Blakeley, R.R. Friedl, J.S. Francisco, R. Liu and S.P. Sander," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 308-319 (2000).

$ClO + HO_2$
Rate Constants
T Dependence
Measurements
Calculations

84729. Dobis, O., and S.W. Benson, "Kinetic Study of the Reaction of Hydrogen Atoms with Molecular Chlorine at Millitorr Pressures," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 777-782 (2000).

$H + Cl_2$
Rate Constants
T Dependence

84730. Wingen, L.M., W.S. Barney, M.J. Lakin, T. Brauers and B.J. Finlayson-Pitts, "A Unique Method for Laboratory Quantification of Gaseous Nitrous Acid (HONO) Using the Reaction $HONO + HCl \rightarrow ClNO + H_2O$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 329-335 (2000).

HONO + HCl
Rate Constant
HONO Calibration Method
Conversion/NOCl Monitoring

84731. Wallington, T.J., K.W. Jucks and G.S. Tyndall, "Upper Limits for the Gas Phase Reaction of H_2O_2 with O_3 and NO: Atmospheric Implications," *Int. J. Chem. Kinet.* 30, 707-709 (1998).

$H_2O_2 + NO$
$H_2O_2 + O_3$
Rate Constants
Upper Limits

84732. Bacchus-Montabonel, M.C., and D. Talbi, "A Theoretical Treatment of the LiH and BeH Formation through Radiative Association," *J. Mol. Struct.* 463, 91-97 (1999).

Li + H
Be + H
Radiative Association
Rate Constants
Calculations

(84473) Rate Constants, MMT = Methylcyclopentadienyl Manganese Tricarbonyl

MMT + OH, O_3

84733. Becker, K.H., R. Kurtenbach, F. Schmidt and P. Wiesen, "Kinetics of the NCO Radical Reacting with Atoms and Selected Molecules," *Combust. Flame* 120, 570-577 (2000).

$NCO + H,O,O_2$
$NCO + CO,CO_2,H_2$
Rate Constants
Measurements

(84519) $NH_2 + NO$ Reaction Branching Inclusion, Adequacies

$DeNO_x$ Process
Kinetic Modeling

84734. Mueller, M.A., J.L. Gatto, R.A. Yetter and F.L. Dryer, "Hydrogen/Nitrogen Dioxide Kinetics: Derived Rate Data for the Reaction $H_2 + NO_2 = HONO + H$ at 833 K," *Combust. Flame* 120, 589-594 (2000).

$NO_2 + H_2$
Rate Constant
$H_2/NO_2/N_2$
Flow Reactor
Species Profiles
Kinetic Model

84735. Loffler, G., V.J. Wargadalam, F. Winter and H. Hofbauer, "Decomposition of Nitrous Oxide at Medium Temperatures," *Combust. Flame* 120, 427-438 (2000).

Kinetic Modeling
$N_2O + M$
$N_2O + O,H,OH$
Flow Reactor
$N_2O/CH_4,CO,H_2$
Adequacies

84736. Picquet, B., S. Heroux, A. Chebbi, J.-F. Doussin, R. Durand-Jolibois, A. Monod, H. Loirat and P. Carlier, "Kinetics of the Reactions of OH Radicals with Some Oxygenated Volatile Organic Compounds under Simulated Atmospheric Conditions," *Int. J. Chem. Kinet.* 30, 839-847 (1998).

$OH + CH_3OH,C_2H_5OH$
$OH + t\text{-}C_4H_9OCH_3$
$OH + CH_3COOR$
$R = C_2\text{-}C_4$ Alkyls
Rate Constants

84737. Baxley, J.S., and J.R. Wells, "The Hydroxyl Radical Reaction Rate Constant and Atmospheric Transformation Products of 2-Butanol and 2-Pentanol," *Int. J. Chem. Kinet.* 30, 745-752 (1998).

$OH + 2\text{-}C_4H_9OH$
$OH + 2\text{-}C_5H_{11}OH$
Rate Constants

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$OH + Cl_2$
$OH + Br_2$
$OH + I_2$
Rate Constants
T Dependences

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$O_2 + Ar$
$O + O + Ar$
Rate Constants
3000-4500 K
Shock Tube

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$O_3 + CH_3COC_2H_3$
$O_3 + CH_2C(CH_3)CHO$
$O_3 + CH_2C(CH_3)COOH$
$O_3 + C_2H_3COOH$
Rate Constants

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O_3+RH
Rate Constants
c-$C_nH_{n-1}(CH_2)$
n=3-6
$C_3H_4Cl(CH_3)$
$C_4H_5Cl(CH_3)$
Measurements

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Si+HCl
Rate Constants
T Dependence
Shock Tube
Measurements

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SiH_2+CH_4
$SiH_2+Si(CH_3)_4$
Rate Constants
Insertion Barriers

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Kinetic Modeling
$SiH_4/H_2/O_2$
Ignition Improver
Data Comparisons

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$Zr+C_2H_4,C_2D_4$
$Zr+C_3H_6,C_3D_6$
Rate Constants
H_2 Elimination

37. PHOTOLYSIS/MPD

(See also Section 38 for Photolytic Product Distributions)

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IR MPA
Diatomics
Intense Laser
Field Effects

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IR MPD
Diatomics
Circularly
Polarized
Chirped Laser
Pulse Effects

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$Ba.FCH_3+h\nu$
Cluster Spectroscopy
Ba*,BaF*
Product Channels
Dynamics

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$CH_2N + h\nu$
Product H Energies
Mechanisms

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$CH_3I + h\nu$
Alignment Effects
Fragment Velocities

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$CH_3I + h\nu$
$CD_3I + h\nu$
Photodissociation Dynamics
$I(^2P_{1/2})$ Yields
Calculations

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$C_2H_2 + h\nu$
$C_2H(A\text{-}X)$
$C_2H_2^+(\nu_{c\text{-}c})$
Assessment

(84699) 193 nm Quantum Yields

$CH_2CO + h\nu$

(84781) Photoisomerization Measurements

$C_4H_4(CHO)_2 + h\nu$

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$CH_3C_6H_4Br + h\nu$
Br Product Energies
Channels
Mechanism

(84552) fs Photoionization, Fragmentation, Mass Analysis

$C_{60} + h\nu$

84754. Orel, A.E., Y. Zhao and O. Kuhn, "Laser Driven Ground State Photodissociation of $HCo(CO)_4$: An ab Initio Quantum Molecular Dynamics Approach," *J. Chem. Phys.* 112, 94-100 (2000).

MPD
$CoH(CO)_4$
Dissociation/
IVR
Competitive
Channels
Modes

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$Fe(CO)_5 + h\nu$
fs Excitation
Fragments
Energies
Model

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$HCl + h\nu$
$Cl(^2P_{1/2,3/2})$ Product
Branching Ratios
Dependences
State Interaction
Effects

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HNCO + hν
P.E. Surfaces
S_1/S_0 Internal Conversion Role

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ICN + hν
fs Spectroscopy
Fragment Monitoring
Wavepacket Mapping

(84473) Absorption Cross Sections, Photolysis Rates, MMT = Methylcyclopentadienyl Manganese Tricarbonyl

MMT + hν

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N_2O + hν
$O(^1D)$,N_2 Products
^{15}N Isotopic Effects

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N_4^+
Photodissociation Dynamics
$N_2^+(A,X)$ Channels
Beam/Mass Analysis

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RbI + hν
Circularly Polarized UV
$Rb(^2P_{1/2}, ^2S_{1/2})$ Fragments

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$SiH_3(CHCHCl)$ + hν
HSiCl*(v,J)Product
LIF
Ar Quenching Rate Constant

(84419) M = Ti,Zr,Hf, CVD Laser Photolysis, TiN*, ZrN* Emission

$M(N(C_2H_5)_2)_4$ + hν

38. REACTION PRODUCT-ENERGY DISTRIBUTIONS

(See also Section 37 for Product Distributions and Section 40 for Theoretically Calculated Reaction Product Distributions)

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IR Chemiluminescence
Reaction Products
Rate Constants
Sensitivities
Review

(84725) Product Distributions, $Cl + CH_3CHO$

HCl(v)

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NH_2(A,v,J)
Product Energy Distributions
$NH_3 + h\nu$
FTIR Analysis

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N_2^+(v,N)
Product Distribution
$N_2 + h\nu$
$N_2O + h\nu$
UV Photoionization

(84633) Product Distribution, $O(^1D) + CH_4$, C_2H_6, C_3H_8, Collision Energy Effects

OH(v=0,1)

84766. Geiser, J.D., S.M. Dylewski, J.A. Mueller, R.J. Wilson, R. Toumi and P.L. Houston, "The Vibrational Distribution of $O_2(X^3\Sigma_g^-)$ Produced in the Photodissociation of Ozone between 226 and 240, and at 266 nm," *J. Chem. Phys.* 112, 1279-1286 (2000).

O_2(v≥26)
Product Yields
$O_3 + h\nu$
226-240,266 nm

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$S(^1D_2)$
Product Orientation
OCS + hν
2-D Mapping

39. UNIMOLECULAR PROCESSES

(See also Section 36 for Unimolecular Rate Constants and Section 40 for Reaction Dynamics)

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Unimolecular Rate Constants
Fall-off Behavior
Formalism

(84933) Isomerization, Isomeric Geometries, Calculations

BNO

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Unimolecular Dissociation
$CF_3Br + Kr$
Rate Constant

84770. Valachovic, L.R., M.F. Tuchler, M. Dulligan, T. Droz-Georget, M Zyrianov, A. Kolessov, H. Reisler and C. Wittig, "Photoinitiated H_2CO Unimolecular Decomposition: Accessing H + HCO Products via S_0 and T_1 Pathways," *J. Chem. Phys.* 112, 2752-2761 (2000).

Unimolecular Dissociation
HCHO
H/HCO Channel
Pathways
Energies

(84939)	M=C, Si, Ge, Sn, Pb Isomers, Structural Calculations, Geometries, Energies, Isomerization	MH_2O_2
84771.	Votsmeier, M., S. Song, D.F. Davidson and R.K. Hanson, "Shock Tube Study of Monomethylamine Thermal Decomposition and NH_2 High Temperature Absorption Coefficient," *Int. J. Chem. Kinet.* 31, 323-330 (1999).	Unimolecular Dissociation CH_3NH_2+M Rate Constants Shock Tube NH_2(597.4 nm) Absorption Coefficient
84772.	Votsmeier, M., S. Song, D.F. Davidson and R.K. Hanson, "Sensitive Detection of NH_2 in Shock Tube Experiments Using Frequency Modulation Spectroscopy," *Int. J. Chem. Kinet.* 31, 445-453 (1999).	Unimolecular Dissociation CH_3NH_2+M Rate Constant NH_2 Monitor
84773.	Gowenlock, B.G., and L. Batt, "The Isomerization of Nitrosomethane to Formaldoxime," *J. Mol. Struct.* 454, 103-104 (1998).	Isomerization CH_3NO/CH_2NOH Channels Energies
84774.	Martinez-Nunez, E., and S.A. Vazquez, "Further Dynamical Studies of the Dissociation and Elimination Reactions of Methyl Nitrite," *J. Chem. Phys.* 111, 10501-10510 (1999).	Unimolecular Dissociation CH_3ONO Channels Rate Constants Calculations
84775.	Huybrechts, G., and G. Van Assche, "Pyrolysis of 1-Chloro-1,1-difluoroethane: Considerations about Its Molecular Nature," *Int. J. Chem. Kinet.* 31, 283-289 (1999).	Unimolecular Dissociation CF_2ClCH_3 HCl Product Dynamics
84776.	Tsang, W., and A. Lifshiftz, "Kinetic Stability of 1,1,1-Trifluoroethane," *Int. J. Chem. Kinet.* 30, 621-628 (1998).	Unimolecular Dissociation CF_3CH_3 Rate Constants T Dependence Shock Tube
84777.	Martinez-Nunez, E., and S.A. Vazquez, "Rotational Effects in the Unimolecular Dissociation of the Acetyl Radical," *Chem. Phys. Lett.* 316, 471-476 (2000).	Unimolecular Dissociation CH_3CO Rotational Effects RRKM Analysis

84778. Hou, H., B. Wang and Y. Gu, "Decomposition and Isomerization of the CH_3CHClO Radical: ab Initio and RRKM Study," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1570-1575 (2000).

Unimolecular Dissociation
CH_3CHClO
12 Channels
Rate Constants
Calculations

84779. Hou, H., B. Wang and Y. Gu, "Ab Initio and RRKM Studies of the Unimolecular Reactions of CH_2XCHFO(X=H,F) Radicals," *Phys. Chem. Chem. Phys.* 2, 61-65 (2000).

Unimolecular Dissociation
CH_3CHFO
CH_2FCHFO
Channels
RRKM Theory
Rate Constants

84780. Kirchner, F., A. Mayer-Figge, F. Zabel and K.H. Becker, "Thermal Stability of Peroxynitrates," *Int. J. Chem. Kinet.* 31, 127-144 (1999).

Unimolecular Dissociation
RO_2NO_2
9 Peroxynitrates
Rate Constants
Lifetimes

84781. Klotz, B., I. Barnes and K.-H. Becker, "Kinetic Study of the Gas Phase Photolysis and OH Radical Reaction of E,Z- and E,E-2,4-Hexadienedial," *Int. J. Chem. Kinet.* 31, 689-697 (1999).

Isomerization
$C_4H_4(CHO)_2 + h\nu$
$C_4H_4(CHO)_2 + OH$
Rate Constants

84782. Chuchani, G., A. Rotinov and R.M. Dominguez, "The Kinetics and Mechanisms of Gas Phase Elimination of Primary, Secondary, and Tertiary 2-Hydroxyalkylbenzenes," *Int. J. Chem. Kinet.* 31, 401-407 (1999).

Unimolecular Dissociation
$C_6H_5CH_2CH_2OH$
$C_6H_5CH_2CH(OH)CH_3$
$C_6H_5CH_2C(CH_3)(OH)CH_3$
Rate Constants
Products

84783. Amatatsu, Y., "Ab Initio Study on the Electronic Structures of Stilbene at the Conical Intersection," *Chem. Phys. Lett.* 314, 364-368 (1999).

Photoisomerization
$C_6H_5CHCHC_6H_5$
Conical S_1/S_0
Intersection
Mechanism

84784. Justum, Y., F. Gatti and X. Chapuisat, "One-Dimensional Quantum Description of the Bending Vibrations of HCN/CNH," *J. Mol. Struct.* 453, 131-140 (1998).

Isomerization
HCN/HNC
Bending
Vibrations
Calculations

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Isomerization
HNC/HCN
IVR Process
Reaction Path
Energies

84786. Jursic, B.S., "Ab Initio and Density Functional Theory Studies of the Potential Energy Surface of the LiNC→LiCN Isomerization," *J. Mol. Struct.* 428, 41-47 (1998).
Isomerization
LiNC/LiCN
P.E. Surface
Energy Barrier

84787. Arranz, F.J., F. Borondo and R.M. Benito, " Transition from Order to Chaos in a Floppy Molecule: LiNC/LiCN," *Chem. Phys. Lett.* 317, 451-457 (2000).
Isomerization
LiNC/LiCN
Order/Chaos
Theory

84788. Mestres, J., M. Fores and M. Sola, "Exploring the Possibility of a Bimolecular Reaction Channel for the F_2SS/FSSF Rearrangement Process," *J. Mol. Struct.* 455, 123-129 (1998).
Isomerization
S_2F_2/FSSF
Bimolecular
Channel
Energies

84789. Jursic, B.S., "Density Functional Theory and Quadratic Complete Basis Set ab Initio Studies of the HNSi to HSiN Isomerization and Hydrogen Insertion Reactions with Further Isomerizations of the Insertion Products," *J. Mol. Struct.* 460, 11-18 (1999).
Isomerization
SiNH/HSiN
$HSiNH_2$/$HNSiH_2$
Stabilities

84790. Kwon, O., and Y. Kwon, "Theoretical Study for the HNSi-HSiN Isomerization: ab Initio and DFT Calculations," *J. Mol. Struct.* 460, 213-220 (1999).
Isomerization
SiNH/HSiN
Structures
Frequencies
Barrier Height

40. CHEMICAL DYNAMICS - THEORY

(See also Section 37 for Photodissociation Dynamics)

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Reaction Dynamics
Rate Constants
P.E. Curve Crossings
Quantum Effects
Analysis

84792. Wang, H., M. Thoss and W.H. Miller, "Forward-Backward Initial Value Representation for the Calculation of Thermal Rate Constants for Reactions in Complex Molecular Systems," *J. Chem. Phys.* 112, 47-55 (2000).
Reaction Dynamics
Rate Constants
Formalism

84793. Zuckerman, D.M., and T.B. Woolf, "Dynamic Reaction Paths and Rates through Importance-Sampled Stochastic Dynamics," *J. Chem. Phys.* 111, 9475-9484 (1999).
Reaction Dynamics
Rates
Average Paths
Formulation

84794. Yarkony, D.R., "On the Adiabatic to Diabatic States Transformation Near Intersections of Conical Intersections," *J. Chem. Phys.* 112, 2111-2120 (2000).
Reaction Dynamics
Conical
Intersection
Representations

84795.	Gimenez, X., F. Huarte-Larranaga, X. Grande, Y. Quiros, M. Alberti and A. Aguilar, "Cross Sections Exhibiting Quantum Resonances: The B+OH Case," *J. Mol. Struct.* 463, 65-74 (1999).	Reaction Dynamics B+OH Cross Sections P.E. Surface Structures
84796.	Collins, M.A., and D.H. Zhang, "Application of Interpolated Potential Energy Surfaces to Quantum Reactive Scattering," *J. Chem. Phys.* 111, 9924-9931 (1999).	Reaction Dynamics $BeH+H_2$ P.E. Surface Interpolation Method
84797.	Hansen, J.C., Y. Li, Z. Li and J.S. Francisco, "On the Mechanism of the BrO+HBr Reaction," *Chem. Phys. Lett.* 314, 341-346 (1999).	Reaction Dynamics BrO+HBr OH+HCl Energies Barriers
84798.	Talbi, D., "An Extensive ab Initio Study of the $C+NH_2$ and $N+CH_2$ Reactions in Relation to the HCN/HNC Space Abundance Ratios," *Chem. Phys. Lett.* 313, 626-632 (1999).	Reaction Dynamics $C+NH_2$ $N+CH_2$ HCN,HNC Product Channels Zero Barriers
84799.	Jursic, B.S., "Theoretical Study of the Fluorine Effect on the Methylene Insertion Reaction in the Hydrogen Molecule, Hydrogen Fluoride and the Fluorine Molecule," *J. Mol. Struct.* 467, 103-113 (1999).	Reaction Dynamics CF_2+F_2,HF,H_2 CH_2+F_2,HF,H_2 Insertion Barriers, Energies ^{1,3}Energy Gap
84800.	Francisco, J.S., "Coupled Cluster and Second-Order Moller-Plesset Perturbation Studies of the Mechanism of the Gas Phase Atom-Radical Reaction of Atomic Hydrogen with CF_2 Radical," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1499-1504 (2000).	Reaction Dynamics CF_2+H Channels Energy Barriers
84801.	So, S.P., "A Gaussian-2 Molecular Orbital Study of the Reaction of CF_3 with NO_2," *Chem. Phys. Lett.* 313, 307-312 (1999).	Reaction Dynamics CF_3+NO_2 Channels Energies
84802.	East, A.L.L., and W.D. Allen, "Comment on 'High Level ab Initio and Density Functional Study of the CH+NO Reaction Product Branching,'" *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1362 (2000).	Reaction Dynamics CH+NO Product Branching Channels Energies
84803.	Jursic, B.S., "Response to Comment on 'High Level ab Initio and Density Functional Study of the CH+NO Reaction Product Branching,' [*J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1362 (2000)]," *ibid.* 104, 1363-1364 (2000).	Reply

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Reaction Dynamics
Rate Constant
Predictive Method
Tunneling
CHF_3,CH_3F+H
CH_2F_2+H

84805. Del Rio, E., R. Lopez, M.I. Menendez and T.L. Sordo, "A Theoretical Study of the Reaction of HCO^+ with C_2H_2," *J. Computat. Chem.* 21, 35-42 (2000).

Reaction Dynamics
$HCO^+ + C_2H_2$
Channels
$C_3H_3^+$,$C_2H_3^+$
Products
Energetics

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Reaction Dynamics
CH_2Cl+CH_3F
C_5H_8 Isomerization
$OH+CH_4$
P.E. Surface
Generating Algorithm

84807. Aplincourt, P., and M.F. Ruiz-Lopez, "Theoretical Study of Formic Acid Anhydride Formation from Carbonyl Oxide in the Atmosphere," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 380-388 (2000).

Reaction Dynamics
$CH_2OO+HCHO$
$CH_2OO+HCHO+O_2$
$CH_2OO+HCOOH$
Energetics
$(HCOO)_2O$
Formation

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Reaction Dynamics
CH_3+Organics
Rate Constants
Structure
Correlation
Predictor
191 Reactions

84809. Jursic, B.S., "A Density Functional Theory Study of the Proton Abstraction from Methane with Triplet Oxygen: An Example of a Very Difficult Computational Problem," *J. Mol. Struct.* 427, 137-142 (1998).

Reaction Dynamics
CH_3+O_2
HO_2 Product
Channel
DFT Accuracies

84810. Jursic, B.S., "Ab Initio and Density Functional Theory Computational Studies of the $CH_4+H \rightarrow CH_3+H_2$ Reaction," *J. Mol. Struct.* 430, 17-22 (1998).

Reaction Dynamics
CH_4+H
Energy Barrier
DFT Methods

84811. Zhang, D.H., and S.-Y. Lee, "Effects of Reagent Rotation and the Accuracy of the Centrifugal Sudden Approximation in the H_2+CN Reaction," *J. Chem. Phys.* 112, 203-211 (2000).

Reaction Dynamics
$CN+H_2$
Cross Sections
Rotational Effects

84812. Jursic, B.S., "Ab Initio and Density Functional Theory Study of the Cyanide Radical Hydrogen Abstraction from Hydrogen Molecules," *J. Mol. Struct.* 428, 55-59 (1998).

Reaction Dynamics
$CN + H_2$
TS Structure
Energies
Calculations

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Reaction Dynamics
$3\ C_2H_2/C_6H_6$
Transition States
Energies
Activation Energy

84814. Sakai, S., "Theoretical Analysis of Concerted and Stepwise Mechanisms of Diels-Alder Reaction between Butadiene and Ethylene," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 922-927 (2000).

Reaction Dynamics
$C_2H_4 + C_4H_6$
Channels
Energy Barriers

84815. Good, D.A., and J.S. Francisco, "Tropospheric Oxidation Mechanism of Dimethyl Ether and Methyl Formate," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1171-1185 (2000).

Reaction Dynamics
$(CH_3)_2O/O_2$
$HCOOCH_3/O_2$
Channels
Energetics

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Reaction Dynamics
$Ca(^1D_2) + HCl$
$Ca(^1D_2) + HBr$
Chemiluminescence
CaCl(A),CaBr(B,A)
Products
Cross Section
Dependences

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Reaction Dynamics
$Cl + CH_2CO$
Rate Constants
P.E. Surface
Channels

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$Cl + HCOOCH_3$
H Abstraction
Dominance

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$Cl + HCl$
Cl Exchange
Efficiencies
Nonadiabatic
Role

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$Cl+H_2$
Rate Constant
P.E. Surface
Energy Barrier

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Reaction Dynamics
Cl^-+CH_3Br
Barrier Recrossings
Calculations

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$D+H_2$
Rate Constant
Wavepacket
Formalism

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D^++H_2
Channels
Calculations

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$F+H_2$
Spin Contamination
Effects
Barrier Height

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Reaction Dynamics
$F+H_2$
State Selective
Forward Scattering
Calculations

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$F^-(H_2O)+CH_3Cl$
Channels

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$H+^{1,3}CO$
Association
DFT Calculations

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Reaction Dynamics
$H+D_2(v=0,1)$
Cross Sections
Comment

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Reaction Dynamics
H + HOD
Channels
Isotope Effects

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$H + H_2$
P.E. Surface
Energy Barrier
H Abstraction
Channel

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Reaction Dynamics
$H + H_2O$
Rate Constants
Model

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Reaction Dynamics
$H + N_2H_2$
$OH + CH_4, C_2H_6$
Transition States
Methods
Adequacies

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Reaction Dynamics
H,D,Mu + O_2
Rate Constants
RRKM Theory
Tunneling
Calculations

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HD^+(v=0-4,J=0-3) + He
Branching Ratios
Calculations

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Reaction Dynamics
HFCO + H,OH
Channels
Energy Barriers
DFT Methods

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Reaction Dynamics
HNCO + N
Rate Constants
NCO Product

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Reaction Dynamics
$HNO + NO_2$
P.E. Surfaces
Channels
Rate Constant

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Reaction Dynamics
$HOSO_2+O_2$
Energetics
SO_3/HO_2 Channel

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Reaction Dynamics
H_2O,SF_6
N_2,NaCl
Dissociation
Vibrational
Excitation
Electric Fields
DFT

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Reaction Dynamics
H_2S+H
Rate Constants
Non-Arrhenius
Behavior

(84627) Reaction Dynamics, VTST, Rate Constants, Nonadiabatic Transitions Role

$N(^2D)+C_2H_2,C_2D_2$

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Reaction Dynamics
NH_2+CH_4,H_2
NH_2+H_2O,NH_3
Rate Constants
D-Substitution
Effects

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Reaction Dynamics
$O+CH_4$
Barrier Height
Stationary Points
Transition States

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$O+CH_4$
P.E. Surface
Rate Constants
Product Energies
Reactant
Energy Effects

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Reaction Dynamics
$O+CH_4$
Reduced
Dimensionality
Model

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Reaction Dynamics
O + HCl
P.E. Surface Calculations

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Reaction Dynamics
O + HCl
Rate Constants
VTST

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Reaction Dynamics
O + HCl
Rate Constants
Rotational Effects

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Reaction Dynamics
$O+OH/O_2+H$
HO_2* Transition State
Angular Momentum
Minor Role

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Reaction Dynamics
$O(^1D)+HCl$
Channels
Products

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Reaction Dynamics
$O^+ + H_2$
Energies
DFT Methods

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$O^- + MH_n$
M = Li,Be,B, C,N,O,F
Stable Complex Structures

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Reaction Dynamics
$OH+CH_4$
$OH+C_2H_6$
Energy Barriers

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Reaction Dynamics
OH + CO/HOCO*
H_2O Effects
Stabilities

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Reaction Dynamics
OH + RH
57 Unsaturated HC
OH + M
312 Reactions
Rate Constants
Correlation
Predictor

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$OH + C_3H_6$
Transition States
Channels
Mechanism

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Reaction Dynamics
$OH + Cl_2$
Reactant Energy
Effects

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Reaction Dynamics
$O_2^- + O_2$
Electron Transfer
Transition State
Rate Constant

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Reaction Dynamics
Zn*,Cd*,Hg* + CH_4
Zn*,Cd*,Hg* + SiH_4
(^{3}P) State
Insertion

41. CHEMICAL KINETICS - GENERAL

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Air Breakdown
Electric Field
NO Effects

(84487) H_2/Ar Discharge, Efficiencies

CCl_2F_2 Destruction

(84569) High Rotational Excitation, Cooled Discharge, FTIR Spectra

CO(v≤6),J

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CHCCl + O_2
Major Products

(84406) Air Mixture, Destruction Efficiencies, Products

$C_2HCl_3 + e^-$

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C_2H_2/N_2
Microwave Discharge
Nitro-organic Products
Analysis

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$CH_3CHO(S_1)$
State Resolved Dissociation
CH_3/HCO Channel Measurements

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$RR'O_2$
Cyclic Peroxide Formation
Chemiluminescence
Review

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$(CF_3)_2CO + CH_2O_2$
$CH_3CHO + CH_2O_2$
Relative Reactivities
C_2H_4/O_3

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$C_3H_7OH + OH$
Product Yields

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$C_4H_6 + NO_3$
$C_4H_6 + OH$
Products
Yields
Mechanisms

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c-$C_4H_8O_2 + OH(NO_x)$
Kinetic Mechanism Sensitivity Analysis

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$C_4H_9SH + H,D$
Product Channels
Mechanism

(84490) Ultrasonic/O_3 Destruction Method, Contaminated Water

t-$C_4H_9OCH_3/H_2O$

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n-$C_4H_9OCH_3 + OH$
i-$C_3H_7OC_2H_4OH + OH$
Product Yields
Channels

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t-$C_4H_9OCH_3/O_2$
t-$C_4H_9OC_2H_5/O_2$
n-C_7H_{16}/Ether
Mixtures
Stirred Reactor
Measurements
Modeling

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C_6H_6+OH
Product Yields
C_6H_5OH,HCOOH
Benzoquinone
Carbonyls

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$(CH_3OCOCH_2)_2CH_2+OH$
Products
Yields

(84624) $Hg(^3P_1)+HCl$, Matrix Study, FTIR Spectra

HHgCl Product

(84517) Combustion Conditions, Catalytic Effects

NO/NO_2
Conversions

(84644) O_2(F,E-X), 113-130 nm Oscillator Strengths, Quantum Yield Dependences

$O(^1D)$ Product

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SF_6/Air
Discharges
SOF_2,SOF_4
Product FTIR
Analysis

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Y+HCHO
Crossed Beams
Product Channels
D_0(YCHO)

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$Y+C_2H_6$
Crossed Beams
C_2H_4,H_2
Product Channels
Energies

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Laser
Attosecond
Pulse Generation
Method

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Laser Ablation
C(s)/Vacuum
C(s)/He,N_2
Spectral Emissions
CN*

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Laser Reaction Control
Phase Shift
Time Delays
Theoretical Analysis

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Laser Control
H-Transfer
$CH_2(CHO)_2$
Pulse Sequence Method

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ps Laser Control
$HONO_2$
Dissociation Channels
Modeling

43. P.E. CURVES/SURFACES/ENERGY LEVELS

(See also Section 26 for Spectral Aspects, Section 40 for Reaction P.E. Surfaces and Section 44 for Structure Calculation Surfaces)

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Vibrational Energy Levels
C_2H_2,HCN
H_2O,H_3^+
Calculations

84882. Viel, A., and C. Leforestier, "Six-Dimensional Calculation of the Vibrational Spectrum of the HFCO Molecule," *J. Chem. Phys.* 112, 1212-1220 (2000).

Vibrational Energy Levels
HFCO
$\leq$5000 cm^{-1}
Calculations

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Vibrational Energy Levels
cis-,*trans*-HOCO
Calculations

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HOCl
Vibrational Spectrum
Levels
P.E. Surface

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v,J Levels
H_2O
P.E. Surface
Calculations
Erratum

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Rovibrational
Energy Levels
H_3^+
New Global
P.E. Surface
Calculations

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Na($5^2S_{1/2}$)
Hyperfine
Splitting
Measurement

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Rovibrational
Energy Levels
O_3
Calculations
Band Centers

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P.E. Surfaces
AlO
Low-lying States
Spectral Constants
PES,AlO^-

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P.E. Curves
BeOH,MgOH
$BeOH^+$,$MgOH^+$
Low-lying States
Energies

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P.E. Curve
$Be_2(X)$
$CH_2(^1A_1$-$^3B_1)$
Energy Splitting
Calculations

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P.E. Curve
Be_2
Spectral Constants
D_0

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P.E. Curves
Be_2
Low-lying States
(B-A′) Laser
Excitation Spectra
Constants

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P.E. Curves
CH
15 States
Spectral Constants
T_e, D_e
Calculations

84895. Braunstein, M., and J.W. Duff, "Electronic Structure and Dynamics of $O(^3P)+CO(^1\Sigma^+)$ Collisions," *J. Chem. Phys.* 112, 2736-2745 (2000).

P.E. Surfaces
CO+O
Data Fitting
Transition State
Geometries

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P.E. Surface
CO/OH
Formalism

84897. Okada, K., and S. Iwata, "Accurate Potential Energy and Transition Dipole Moment Curves for Several Electronic States of CO^+," *J. Chem. Phys.* 112, 1804-1808 (2000).

P.E. Curves
CO^+
Low-lying States
Transition Moments
B,A-State
Lifetimes

84898. Zuniga, J., A. Bastida, M. Alacid and A. Requena, "Global Potential Energy Surfaces for the CO_2 and CS_2 Molecules," *Chem. Phys. Lett.* 313, 670-678 (1999).

P.E. Surfaces
CO_2, CS_2
Ground State
Calculations

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Intermolecular
Potentials
C_6H_6.Ar
Accuracy
Testing Method

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P.E. Curves
ClF
Low-lying States
Ion Pair States
Spectral Constants

84901. Toniolo, A., M. Persico and D. Pitea, "An ab Initio Study of Spectroscopy and Predissociation of ClO," *J. Chem. Phys.* 112, 2790-2797 (2000).

P.E. Curves
ClO
Low-lying States
A-State
Predissociation
Mechanisms

84902. Meuwly, M., and J.M. Hutson, "Intermolecular Potential Energy Surfaces and Bound States in F-HF," *J. Chem. Phys.* 112, 592-600 (2000).

P.E. Surfaces
F/HF
Well Depth

84903. Dutta, A., J. Bhattacharjee and K.K. Das, "($A^3\Pi_{0+}$-$X^1\Sigma_{0+}^+$) and ($B^3\Pi_1$-$X^1\Sigma_{0+}^+$) Transitions of GaI: An MRDCI Study," *Chem. Phys. Lett.* 314, 347-352 (1999).

P.E. Curves
GaI(B,A-X)
Spectral Constants
Low-lying States
Lifetimes
Calculations

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P.E. Curves
GaP
Low-lying States
Spectral Constants
Lifetimes
Transition Strengths
$D_e(X)$

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P.E. Curves
Ga_2
Low-lying States
Spectral Constants
$D_0(X)$

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P.E. Curves
HCl,DCl($^{1,3}\Pi$)
HCl,DCl($^3\Sigma^+$)
Predissociation
Linewidths
$D^1\Pi$,$d^3\Pi$ States

84907. Huang, Z., and Z.H. Zhu, "Molecular Structure and Analytical Potential Energy Function for the HCl_2^+ (X^1A') System," *J. Mol. Struct.* 448, 17-20 (1998).

P.E. Function
$HCl_2^+(X)$
Spectral Constants
D_e

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P.E. Surface
HOCl
Data Fitted
Accuracy

84909. Bian, W., and H.-J. Werner, "Global ab Initio Potential Energy Surfaces for the ClH_2 Reactive System," *J. Chem. Phys.* 112, 220-229 (2000).

P.E. Surfaces
H_2Cl
$Cl + H_2$
Barrier Height

84910. Kain, J.S., O.L. Polyansky and J. Tennyson, "The Ground State Potential Energy Surface of Water: Barrier to Linearity and Its Effect on the Vibration-Rotation Levels," *Chem. Phys. Lett.* 317, 365-371 (2000).

P.E. Surface
H_2O
Improvements
v,J Energy Levels

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P.E. Surface
H_2O_2, ν_4
Stable
Conformation

84912. Jin, B., H.L. Schmider and D. Wardlaw, "Potential Energy Surfaces for the Colinear H_3^+ System," *Chem. Phys. Lett.* 317, 464-471 (2000).

P.E. Surfaces
H_3^+
2 Lowest
Singlet States
Transition Moments

84913. Cybulski, S.M., and R.R. Toczylowski, "Ground State Potential Energy Curves for He_2, Ne_2, Ar_2, He-Ne, He-Ar and Ne-Ar: A Coupled-Cluster Study," *J. Chem. Phys.* 111, 10520-10528 (1999).

P.E. Curves
He_2, Ne_2, Ar_2
HeNe,HeAr,NeAr
Spectral Constants
D_0
Calculations

84914. Hogreve, H., "Quartet States of He_2^+," *Mol. Phys.* 98, 249-254 (2000).

P.E. Curves
He_2^+
Low-lying
Quartet States
Spectral Constants
D_e

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P.E. Curves
ICl
Low-lying States
Avoided Crossings
Photodissociation
Mechanisms

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P.E. Curves
LiHe(B,A,X)
Spectral Constants
D_e

(84786) P.E. Surface, Isomerization, Energy Barrier

LiNC/LiCN

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P.E. Curves
Li_2^-
Low-lying States
Spectral Constants
D

84918. Sanz, V., A. Aguado and M. Paniagua, "Second-Order Density Functional Calculations of the MgFH Potential Energy Surface," *J. Mol. Struct.* 426, 165-169 (1998).

P.E. Surface
MgFH
Transition State
Energy

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P.E. Curves
MoN
Low-lying States
Spectral Constants
Dipole Moment
D_0

84920. Klos, J., G. Chalasinski, M.T. Berry, R. Bukowski and S.M. Cybulski, "Ab Initio Potential Energy Surface for the He(^{1}S) + NO($X^2\Pi$) Interaction and Bound Rovibrational States," *J. Chem. Phys.* 112, 2195-2203 (2000).

P.E. Surfaces
NO.He($^2A'$,$^2A''$)
Well Depths
v,J Bound States

84921. Theodorakopoulos, G., I.D. Petsalakis and M.S. Child, "An ab Initio Potential Energy Surface and Spectroscopic Constants for the $X^1\Sigma_g^+$ State of NO_2^+," *J. Mol. Struct.* 434, 177-182 (1998).

P.E. Function
$NO_2^+(X)$
Spectral Constants
Frequencies
Calculations

84922. Honjou, N., and E. Miyoshi, "An ab Initio Study on the Electronic Structure of the $3^2\Sigma_u^+$, $3^2\Sigma_g^+$ and $4^2\Sigma_g^+$ States of N_2^+," *J. Mol. Struct.* 451, 41-49 (1998).

P.E. Curves
$N_2^+(3^2\Sigma_u^+)$
$N_2^+(3,4^2\Sigma_g^+)$
r_e,Energies
Avoided Crossings

84923. Kowalczyk, P., W. Jastrzebski, A. Pashov, S. Magnier and M. Aubert-Frecon, "Potential Energies of the $4^1\Pi$ and $5^1\Pi$ States of NaK by Polarization Labeling Spectroscopy and by ab Initio Calculations," *Chem. Phys. Lett.* 314, 47-51 (1999).

P.E. Curves
$NaK(4,5^1\Pi)$
Polarization
Labeling Spectra

84924. Petrov, A.N., and A.I. Panin, "Electronic Structure of the Excimer Emitting Systems of the Type Inert Gas-Alkali Metal: The $HeNa^+$ Cation," *Opt. Spectrosc., Russia* 86, 377-382 (1999).

P.E. Curves
Na^+.He
$1^{1,3}\Sigma^+$,$2^1\Sigma^+$ States
Stabilities
$2^1\Sigma^+$ Lifetime

84925. Lee, H.-S., A.B. McCoy, L.B. Harding, C.C. Carter and T.A. Miller, "An Empirical Potential Energy Surface for the Ne-OH/D Complexes," *J. Chem. Phys.* 111, 10053-10060 (1999).

P.E. Surfaces
OH.Ne(A,X)
OD.Ne(A,X)
Data Fitting

84926. Jursic, B.S., "Potential Energy Surface for H_2Si_2 Isomer Explored with Complete Basis Set ab Initio Method," *J. Mol. Struct.* 459, 221-228 (1999).

P.E. Surfaces
Si_2H_2
Isomers
Stabilities

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P.E. Curve
$Ti_2(X)$
D_e
Calculations

84928. Dai, D., and K. Balasubramanian, "Electronic States and Potential Energy Surfaces of WC_2," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1325-1331 (2000).

P.E. Surfaces
WC_2
Low-lying States
Geometries
Frequencies
Energies

44. ATOMIC/MOLECULAR STRUCTURES

(See also Section 26 for Spectrally Measured Structures)

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Structural
Calculations
Spectral Properties
P.E. Curves
Bibliography
4406 References

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Structural
Calculations
M_2
First Row
Transition Metals
D, r_e

84931. Tsuchiya, T., T. Taketsugu, H. Nakano and K. Hirao, "Theoretical Study of Electronic and Geometric Structures of a Series of Lanthanide Trihalides LnX_3(Ln=La-Lu; X=Cl,F)," *J. Mol. Struct.* 461/462, 203-222 (1999).

Structural
Calculations
MF_3, MCl_3
M=La-Lu
Geometries
Frequencies

84932. Jursic, B.S., "Hybrid Density Functional Theory and Quadratic Complete Basis Set ab Initio Computational Study of Structural Properties, Vibrational Spectra, and Bond Dissociation Energy for Methyl Aluminum and Methyl Gallium," *J. Mol. Struct.* 428, 61-66 (1998).

Structural
Calculations
$AlCH_3$
$GaCH_3$
Geometries
Frequencies

84933. Su, S., "An Electronic Structure Investigation of the BNO-BON-NBO System," *J. Mol. Struct.* 430, 137-148 (1998).

Structural
Calculations
BNO
Isomers
Isomerization
Geometries

84934. Lee, E.P.F., and T.G. Wright, "Geometry, Vibrational Frequencies and Ionization Energies of BeX_2(X=F, Cl, Br and I)," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 974-981 (2000).

Structural
Calculations
BeF_2,$BeCl_2$
$BeBr_2$,BeI_2
Neutrals,Cations
Geometries
Frequencies
IPS

84935. Pacios, L.F., and P.C. Gomez, "Bonding in Bromine Oxides: Isomers of BrO_2, Br_2O_2 and BrO_3," *J. Mol. Struct.* 467, 223-231 (1999).

Structural
Calculations
BrO_2,BrO_3
Br_2O_2
Geometries
ΔH_f

84936. Sendt, K., and G.B. Bacskay, "Spectroscopic Constants of the X($^1A_1$), a($^3B_1$), and A($^1B_1$) States of CF_2, CCl_2, and CBr_2 and Heats of Formation of Selected Halocarbenes: An ab Initio Quantum Chemical Study," *J. Chem. Phys.* 112, 2227-2238 (2000).

Structural
Calculations
CF_2(A,a,X)
CCl_2,CBr_2(A,a,X)
Geometries
Frequencies
ΔH_f(CF_2,CCl_2,CBr_2)
ΔH_f(CHF,CHCl,CFCl)

84937. Wang, X.-G., E.L. Sibert III and J.M.L. Martin, "Anharmonic Force Field and Vibrational Frequencies of Tetrafluoromethane (CF_4) and Tetrafluorosilane (SiF_4)," *J. Chem. Phys.* 112, 1353-1366 (2000).

Structural
Calculations
CF_4,SiF_4
Frequencies
Force Field

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Structural
Calculations
HCHO(A,X)
Geometries
Frequencies
Energies

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Structural Calculations
MH_2O_2
M=C,Si,Ge,Sn,Pb
Isomers
Geometries
Energies
Isomerization

84940. Cabral, B.J.C., "Theoretical Calculations of Molecular Properties of a CFC Substitute: $CHCl_2CF_3$ (HCFC-123)," *J. Mol. Struct.* 452, 117-124 (1998).

Structural Calculations
CF_3CHCl_2
Geometry
Dipole Moment

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Structural Calculations
CF_3OCH_3
$(CHF_2)_2O$
CF_3OCHF_2
Excited State Energies

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Structural Calculations
CF_3COF
CF_3COCl
Frequencies

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Structural Calculations
CH_3CHX
CH_2CH_2X
X=F,Cl,Br
Geometries
Frequencies

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Structures
$C_2H_5NCl_2$
i-$C_3H_7NCl_2$
Geometries
Force Constants
Measurements

84945. Jursic, B.S., "Density Functional Theory Investigation of Physical Properties of the OCCN Radical and the Cation," *J. Mol. Struct.* 460, 207-212 (1999).

Structural Calculations
$OCCN,OCCN^+$
ΔH_f, IP
IR Spectra

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Structural
Calculations
C_3H_3
Frequencies

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Structural
Calculations
c-C_3H_6
c-$C_3H_4D_2$
Geometries
Experimental
Rotational
Constants

84948. Wu, G., C. Van Alsenoy, H.J. Geise, E. Sluyts, B.J. Van der Veken, I.F. Shishkov and L.V. Khristenko, "Acetic Anhydride in the Gas Phase, Studied by Electron Diffraction and Infrared Spectroscopy, Supplemented with ab Initio Calculations of Geometries and Force Fields," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 104, 1576-1587 (2000).

Structural
Calculations
$(CH_3CO)_2O$
Geometries
Frequencies
Electron Diffraction
Measurements

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Structural
Calculations
$C_6H_5NH_2(S_1)$
D Substitution
Isotopomers
Geometries
Frequencies

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Structure
$CH_3C_6H_4NO_2$
Geometry
Measurements
Calculations

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Structural
Calculations
C_{20}
Electronic
Description

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Structural
Calculations
C_{60} ,C_{60}^{6-}
Frequency
Assignments
Data Comparisons

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Structural
Calculations
Cl_2O_2
Isomers
Geometries
Energies

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Structural
Calculations
Cl_2O_3
Isomers
Relative
Stabilities

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Structural
Calculations
Cr_2O_2,Cr_2O_3
Cr_2O_4
Geometries
Frequencies
IR Spectra

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Structural
Calculations
CuH^+
Bond Length
D_0

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Structural
Calculations
FeH_3,ScH_3
TiH_3,VH_3
Geometries
Frequencies
IR Intensities

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Structure
$GaBr_3$, $(GaBr_3)_2$
Geometries
Diffraction
Measurements

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Structural
Calculations
GaP,GaP^-
GaP_2,GaP_2^-
Geometries
Frequencies
Spectral Constants
Low-lying States
EA

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SiF_4
Geometry

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Geometries
Frequencies
Stabilities

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TiCl,TiH,TiH^+
Spectral Constants
D_e

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Relaxation
$C_6H_6(2\nu_{cc})$
IVR Pathways
Modeling

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Vibrational
Relaxation
$HCN^+(v) + He$
$DCN^+(v) + He$
Rate Constants

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$H_2(v=1,J) + H_2$
Calculations

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$H_2 + He$
Forward/Backward
IVR Model
Average Energy
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N_2
Rate Constants
Model

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$N_2(v) + e^-$
T_e(0.1-5 eV)

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Relaxation
$O_2(v \geq 23) + O_2$
Fast Multiquantum
Transitions

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$M = O_3, Rg, O_2, N_2$
Rate Constants

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IVR
$W(CO)_6, \nu_{CO}$
ps Pump/Probe
Collision Free
Decay

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$CN(A, v=3, J) + Ar$
Rate Constants

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Energy Transfer
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Cross Sections
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$C_2H_2(X, v_2=1, J)$
Effects on
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NH(A-X)
ps DFWM
Measurements

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NH(X,v=0,J=3,N=3)
Ne Induced
Rate Constants
SEP Selective Formation Method

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NH_2(A)/Ar
Measurements
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Rotational Energy Transfer
NO(J=1/2)+Ar
Steric Effects
Product J States

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Cross Sections

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48 Molecules
Calculation Method
$\Delta H_{Vaporization}$
C(s),S(s)

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D_0
28 Molecules
9 DFT methods
Comparisons

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G-3 Theory
Accuracies

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$D(MH^+)$
M=Sc thru Zn
Bonding Nature
r_e
Calculations

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ΔH_f, D(MX)
M=B,Al,Ga,In
X=CH_3,Cl,H
n=1-3
Calculations

(84930) First Row Transition Metals, Sc_2 Ti_2, V_2, Cr_2, Mn_2, Fe_2, Co_2, Ni_2 and Cu_2, r_e, Structural Calculations

$D(M_2)$

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ΔH_f
24 Aluminum
Compounds
Calculations

(84236) Equilibrium Calculations, Metal Distributions, Coal Combustion

As,Cd,Hg,Ni
Pb,Se,V,Zn

(84560) B_3N^- Photoelectron Detachment Spectrum, Electronic Structures

EA(B_3N)

(84934) Structural Calculations, Neutrals, Cations, Geometries, Frequencies

IP(BeF_2,$BeCl_2$)
IP($BeBr_2$,BeI_2)

(84892) P.E. Curve, Spectral Constants, Calculations

$D_0(Be_2)$

(84935) Structural Calculations, Geometries

$\Delta H_f(BrO_2,BrO_3)$
$\Delta H_f(Br_2O_2)$

(84936) Structural Calculations, Geometries, Frequencies

$\Delta H_f(CF_2,CCl_2,CBr_2)$
ΔH_f(CHF,CHCl,CFCl)

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ΔH_f
HFCs
Additivity Rule
Deviations

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150 Fluorinated Ethers
Boiling Points
Properties
Alternate Fluorocarbons

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ΔH_f
Hydrocarbon Free Radicals
Semiempirical Estimation Method

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ΔH_{fusion}
Organics
Group Additivity
Estimation Method
1858 Compounds

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D_e, T_e (CH)

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$D(CH_nF_{3-n}SH)$
Calculations

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$CH_2(^1A_1\text{-}^3B_1)$

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IP(i-C_3H_7,t-C_4H_9)
Calculations
Geometries

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$S_{298}(CH_3NO_2)$

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$D(CH_3OCl)$
$D(CH_3OBr)$
$\Delta H_f(CH_2OCl,CH_2OBr)$
Calculations

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$D(CH_3Cl,CH_3Br)$
CH_2X_2, CHX_3
Calculation Methodology

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$D(MOH^+,HMO^+)$
M=C,Si,Ge,Sn
PA Calculations
Structures
Frequencies

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ΔH_f ,$D_0(C_2)$
$\Delta H_f(C_2^+)$
$C^+ + CO$
Reaction
Energy Threshold

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IP,EA(CH_2CN)
$\Delta H_f(ICH_2CN)$
PEPICO Spectra

(84568) $R=C_2H_5$, C_3H_7, C_4H_9 Anion Photoelectron Spectroscopy, Vibronic Structure

ΔH_f ,EA(RO)
D(ROH),$\Delta H_f(RO^{\pm})$

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PA(ROH)
$R=C_2$-C_8 Alkyl
Kinetic Method
Appraisal

(84945) Structural Calculations, OCCN, $OCCN^+$, Infrared Spectra

ΔH_f ,IP(OCCN)

(84575) Photoionization Spectrum, Vibrational Frequencies

IP(C_2H_5SCl)

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IP(C_3H_3)
ZEKE-PES
Spectrum
Frequencies

(84685) $Br + C_5H_{10}$, C_6H_{12} Rate Constants, Temperature Dependences

$\Delta H_f(C_5H_{10}Br)$
$\Delta H_f(C_6H_{12}Br)$

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$\Delta H_f((CH_3)_2CCH(CH_3)_2)$
$\Delta H_f(t\text{-}C_4H_9)$
$CH_3 + (CH_3)_2CCH(CH_3)$
Equilibrium
Constants
Measurements

(84716) $C_6H_5 + CO + Ar$ Rate Constants, RRKM Analysis

$\Delta H_f(C_6H_5CO)$

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IP,EA(C_{60})
Absorption
Spectrum
Calculations

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Cr Compounds
s,l Phases
Thermochemical
Values
Evaluation

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$D_0(CuH^+)$

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(84904)	P.E. Curves, Low-lying States, Spectral Constants, Lifetimes, Transition Strengths, Calculations	D_e(GaP)
(84959)	Structural Calculations, Neutrals, Anions, Geometries, Frequencies, Spectral Constants, Low-lying States	EA(GaP,GaP_2)
(84905)	P.E. Curves, Low-lying States, Spectral Constants	$D_0(Ga_2)$
(84907)	P.E. Function, Spectral Constants, Calculations	$D_e(HCl_2)$
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(84913)	P.E. Curves, Spectral Constants, Calculations	$D_0(He_2, Ne_2, Ar_2)$ D_0(HeNe,HeAr,NeAr)
(84914)	P.E. Curves, Low-lying Quartet States, Spectral Constants	$D_e(He_2^+)$
(84686)	$Br + IBr/I + Br_2$ Rate Constant Measurements	ΔH_f(IBr)
(84916)	P.E. Curves, (B,A,X) States, Spectral Constants, Calculations	D_e(LiHe)
(84917)	P.E. Curves, Low-lying States, Spectral Constants	$D(Li_2^-)$
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(84919)	P.E. Curves, Low-lying States, Spectral Constants, Dipole Moment, Calculations	D_0(MoN)
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(84964)	Structural Calculations, Geometry	$D_0(NH_3)_2$

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$NH_4N(NO_2)_2$
$\Delta H_{sublimation}$
Decomposition
Channels
Calculations

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Thermodynamic
Properties
29 Nitro-Compounds
TNT,RDX,HMX
PETN,NPN,NG

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IP,EA(PF,PF_2)
Calculations

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JANAF Tables
PH(g),PH_3(g)
PN(g)
$Mg_3P_2O_8$(s,l)
Recalculations

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EA(PO_3)
PO_3(A,X)
Frequencies
Energies
PO_3^-,PES

(84411) Calculations

$\Delta H_f(P_2H_n^+)$
n=1-6

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D(SO,SO_2)
DFT
Calculations
Adequacies

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EA(HSO_4,SO_4)
Anion PES
Geometries
Measurements
Calculations

(84614) Rotational Spectrum, Constants

D_e(ScBr)

(84970) Structural Calculations, Spectral Constants

D_e(TiCl)
D_e(TiH,TiH^+)

(84927) P.E. Curve, Calculations

$D_e(Ti_2)$

(84310) Thermodynamic Property Calculations, 0-1500 K

TNAZ

(84874) Y + HCHO Crossed Beams, Product Channels

D_0(YCHO)

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EA(ZrO_2)
ZrO^-,ZrO_2^-
PES Spectra

47. EXPERIMENTAL METHODS

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Alignment
Effects
NaK(D-X)
Polarized Light
Pumping Method

(84407) NO^+/He Drift Tube Calculations

Rotational
Alignment

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Fundamental
Physical Constants
Recommended
CODATA Values